SECONDARY ELECTRON EMISSION FROM MONOCRYSTALLINE METAL AND ALKALI-HALIDE CRYSTALS

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THESIS

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AND ALKALI-HALIDE CRYSTALS

by

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by

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ABSTRACT

This thesis is a computer simulation of secondary electron emission (SEE) from monocrystalline metals and alkali-halides using a modified version of the Harrison, Carlston and Magnuson single collision theory of SEE. Three cases of SEE are investigated: the angular dependence of SEE from Cu bombarded by Ar^+, the dependence of SEE as a function of energy for rare gas ions normally incident on the (100), (110) and (111) faces of metal single crystals, and the dependence of SEE as a function of energy for Ar^+ and Ne^+ ions normally incident on the (100), (110) and (111) faces of KCl. The theory does not accurately describe the angular dependence of SEE for monocrystalline Cu targets, but does accurately predict the modified sec θ dependence found experimentally in polycrystalline studies. For the metal targets, the difference between the theoretical kinetic secondary emission result and the experimental datum is identified as potential secondary emission. The alkali-halide SEE simulation agrees reasonably well with experiment.

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I. INTRODUCTION

Secondary electron emission is the release of electrons from target materials bombarded by primary ions. The first observation of secondary electron emission in 1889 was by Villard who noticed electrons being ejected from the cathode in a discharge tube. Secondary electron mission (SEE) is characterized by the coefficient of ion-electron emission, γ, which is defined as the number of electrons liberated per incident ion.

Secondary electron emission can be produced by two mechanisms, potential emission (PSE) and kinetic emission (KSE). Potential emission arises from the fact that as an ion approaches a target material it may become energetically feasible for a free electron to be emitted from the target surface either by Auger neutralization or Auger recombination. On the other hand, kinetic emission arises from the actual collision between the electrons of the impinging ion and the electrons in the target atom. In general, γ depends primarily upon the PSE mechanism at ion energies below one Kev and the KSE begins to contribute at ion energies above one Kev. Although this is a fairly good rule of thumb, variables such as the work function of the target material, ion charge, surface state of the target, target temperature, and whether the monocrystalline or polycrystalline nature of the target affect the value of the KSE threshold.

Medved et al. [1] have shown that potential emission from Ar^+ and Ar° on Mo increases with energy, with the total SEE at higher energies consisting partly of a KSE component and partly of a PSE component. In general there exists a transition region that is not sharply defined and for this reason it is felt that PSE contributes to secondary emission in the energy range above one Kev, even though the KSE should be the dominant emission mechanism in the one to ten Kev energy range. Both types of emission are investigated in this thesis.

II. STUDY OBJECTIVES

In 1964 Harrison, Carlston and Magnuson [2] proposed a single collision theory of secondary electron emission from monocrystalline target materials in the one to ten Kev primary ion energy range. The original paper develops a theory applicable to monocrystalline targets bombarded by inert gas ion beams directed normal to the (100), (110) and (111) crystal faces. This thesis will extend this theory to explain the following phenomena in the one to ten Kev primary ion energy range:

1. Secondary electron emission from a single crystal plane rotated arbitrarily about a crystallographic axis,
2. Secondary electron emission from metal single crystals, and
3. Secondary electron emission from alkali-halide monocrystals.

III. SECONDARY ELECTRON EMISSION THEORY

Secondary electron ejection mechanisms are either of the potential or kinetic type. Potential ejection can be caused by resonance neutralization, resonance ionization, Auger neutralization, or Auger de-excitation. Kinetic ejection requires the direct transfer of the ion's kinetic energy to the electrons of the target atom. Both mechanisms are discussed below.

Resonance neutralization occurs when it is energetically feasible for an electron in the target material to "tunnel" through its potential barrier and approach the position of the incoming ion. This stage of the process increases the energy of the ion and target atom system by an amount equal to the energy needed to remove an electron from the metal. This energy can range from near zero to ϕ, the work function of the target material. In the second stage of resonance neutralization, the electron and the ion combine, effectively at infinity, to reduce the system energy to an amouht V_i, the ionization potential of the ion. This mechanism is not quite as simple as it seems, since it is affected by the image potential and coulombic forces of the electronic structure of the atoms in the crystal. According to the Franck-Condon principle, the electronic transition of the electron from the target material to the ion can only occur with appreciable probability when the position and velocity

of the ion are not affected by the transition. By this principle we expect a crossover of the initial and final potential energy curves of the system. Taking the image potential into account, resonance neutralization can occur for reasonable separations of ion and target atom when

$$(V_i - V_e) - \phi + I_s < W_a - \phi ,$$

and

$$(V_i - V_e) + I_s > \phi .$$

Therefore $$\phi < (V_i - V_e) + I_s < W_a ,$$

where ϕ is the work function of the target material, V_i, the ionization potential of the ion, V_e, the excitation potential of the primary ion, I_s, the surface image potential and W_a, the initial kinetic energy of the primary ion.

The second possible potential ejection mechanism is resonance ionization which is essentially the reverse process of resonance neutralization. In resonance ionization an excited atom at infinity is ionized into an electron and an ion. The electron then proceeds to the metal surface and occupies any of the unfilled available states above the Fermi level of the metal. As in resonance neutralization, there is a range of ion-target atom separation for which the process is most likely to occur. There is also the possibility that a highly excited atom will be ionized very close to the target surface with a subsequent high probability that a secondary electron will be produced.

Although the above processes are possible, they are not the ones that make the largest contributions to secondary electron emission at low energies. Auger processes, which occur at distances of approach of 3 Å or less, are the primary mechanisms contributing to PSE in the low Kev energy range. These can be summarized as follows [3]:

Auger neutralization:

$$X^+ + ne_m^- \rightarrow X + e^- + (n-2)e_m^- ,$$

and

Auger de-excitation:

$$X^m + ne_m^- \rightarrow X + e^- + (n-1)e_m^- ,$$

where X^+ and X^m refer to the bombarding ion or metastable atom, respectively, and ne_m^- is the number of free electrons initially in the target material. In both cases, the final state of the system is such that a free electron and a neutral atom are produced. Auger neutralization occurs when the energy of the initial system, target and ion, is greater than the resulting system, $X + e^- + (n-2)e_m^-$, at infinite separation. Schematically the process is shown in Figure 1 [3]. Auger de-excitation, on the other hand, involves a metastable atom which approaches the target material. As a result, the initial energy curve, shown in Figure 2 [3], is not modified by an image potential and hence the initial and final energy states never cross.

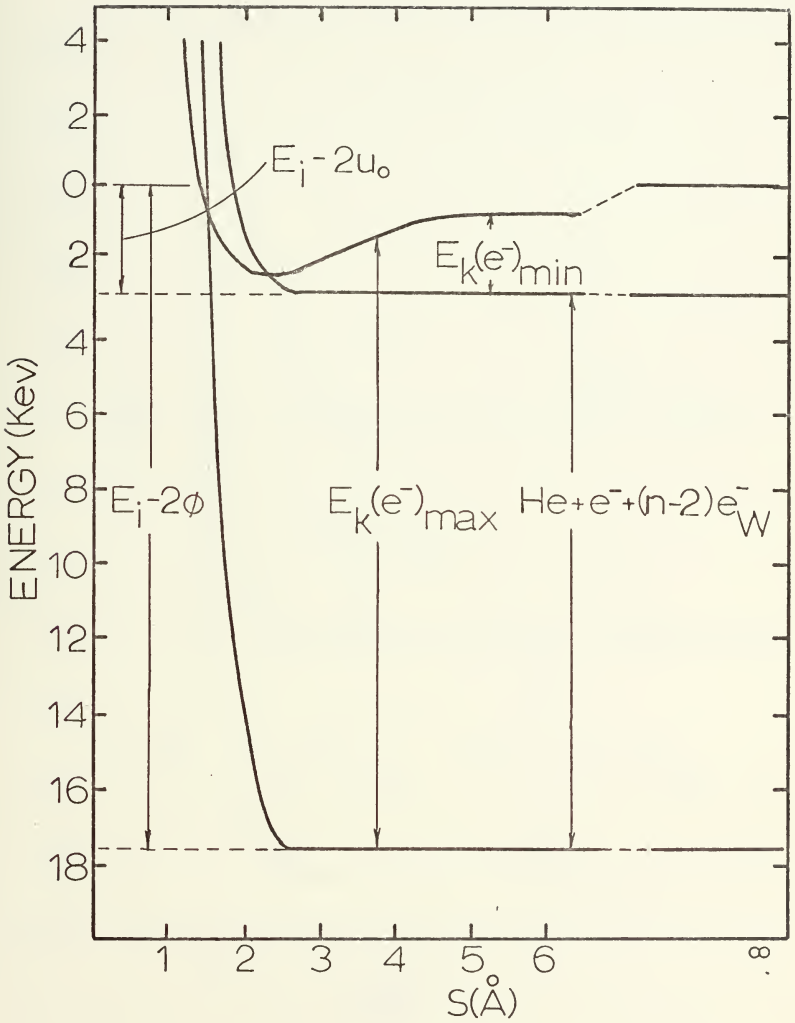

Figure 1. Potential energy diagram for a helium ion as it undergoes Auger neutralization at a tungsten surface (3).

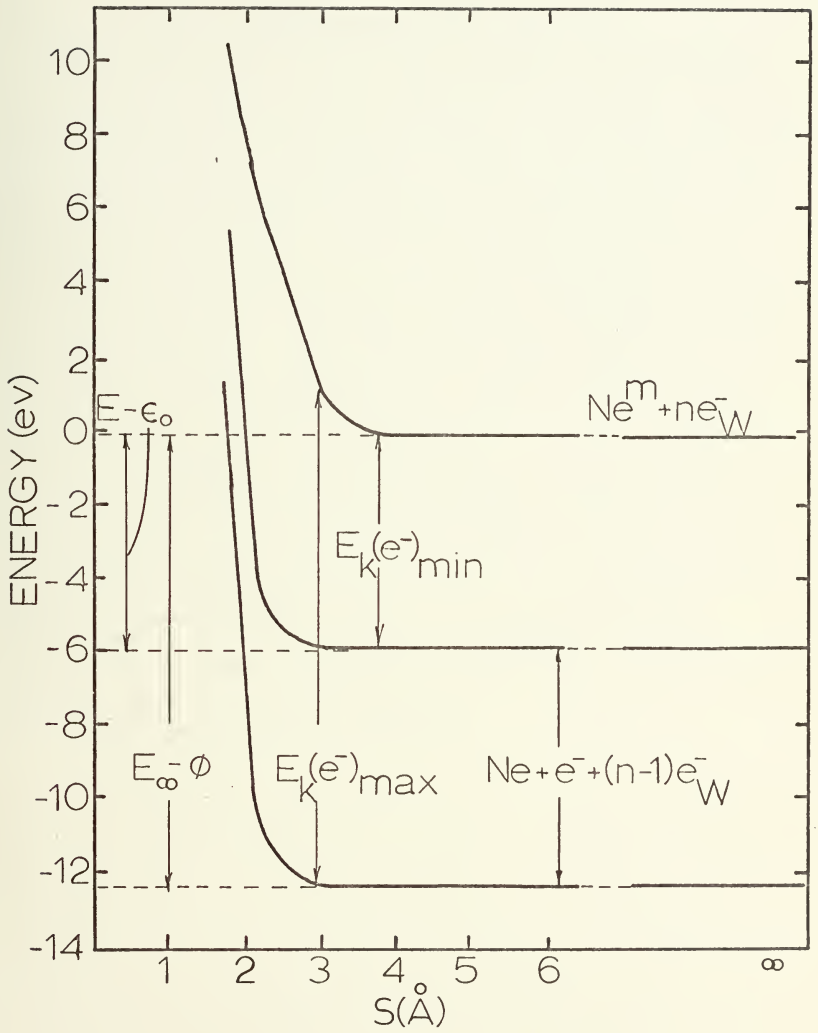

Figure 2. Potential energy diagram for a metastable atom (He) as it undergoes Auger de-excitation at a tungsten surface (3).

These two processes, to a great extent, account for low energy (ev range) secondary electron emission.

Kinetic emission is the result of the direct transfer of the incoming ion's kinetic energy to the atom's electrons. Part of this energy is absorbed in the recoil of the atom, while some of the remaining energy is transferred to the electrons of both the ion and target atom, causing an excitation of both of their electronic structures. As the two nuclei separate, some of the perturbed electrons are liberated as secondary electrons. The ion and recoiling target atom are slowed down within the crystal structure of the target material and are likely to undergo Auger neutralization or de-excitation. If this process occurs sufficiently close to the surface of the target material, there is a probability that these electrons also will escape from the target materials surface and contribute to kinetic secondary electron emission.

IV. THEORIES CONCERNING SECONDARY ELECTRON EMISSION

A. THEORY OF PARILIS AND KISHINEVSKII

Of all the theories proposed to explain kinetic secondary electron emission, the theory of Parilis and Kishinevskii (PK) seemed to be one of the most promising [4]. PK divided the secondary electron emission problem into two separate subproblems which were analyzed separately and subsequently collated to develop the theory of KSE. These two subproblems included:

1. The search for a sufficiently effective mechanism of transfer of the kinetic energy of a moving particle to the (target) electron; and
2. The description of the yield of excited electrons from the target. [4]

PK assumed that the solution to the first problem was of the form proposed by O. B. Firsov for inelastic scattering of ion-atom collisons in the Kev range [5]. Secondly, PK visualized the secondary electron emission process as one in which the primary ion ionizes many atoms as it progresses along its trajectory in the crystal. Electrons produced in this manner, or by further ionization of the primary ion, then proceed to the surface suffering collisions and energy losses as well as possible capture in route. The combination of the electron production phase and the electron escape phase then yields the KSE from the crystal.

The actual collision between the ion and the atom was seen by PK as being accompanied by an overlap of the

electron shell structure of the two collision partners, during which time there occurred an electronic interaction. Energy was transferred between colliding particles, exciting their electrons to a higher energy state. To calculate this excitation energy, a statistical picture of the electron distribution of the particles was used. The theoretical relationship, based on the Thomas-Fermi (TF) model of the atom, leads to the following formula for the energy transferred between the colliding particles:

$$E = \frac{m^2e^2}{4\pi^2\hbar^3} \int \left(\int_S \phi^2 \, dS\right) \dot{\underline{R}} \cdot d\underline{R} \, ,$$

where $\underline{R}$ is the radius vector connecting the centers of the colliding particles, S is the surface separating the domain of action for the potential of the two particles, and ϕ is the potential on this surface given by:

$$\phi = \left[\frac{(Z_1 + Z_2)e}{r}\right] \chi \left[\frac{1.13(Z_1 + Z_2)^{1/3}r}{a_{TF}}\right] ,$$

where Z_i is the charge on each particle, $a_{TF} = h^2/me^2$ and χ is the TF screening function [8]. Physically, the interaction can be thought of as analogous to the collision of two tennis balls. As they impact, both deform, with the vector joining their centers being perpendicular to the area S of the plane of interaction which separates them. Obviously the total energy transferred is a function of the relative velocity with which the ion and atom impact and

the electron distribution associated with each. In terms of the tennis ball analogy, the greater the relative impact velocity, the larger the deformed area S, the shorter the radius vector distance $\underline{R}$, and the greater the number of electrons involved.

The analysis was rewritten by PK in terms of the impact parameter associated with the collision. Hence by changing variables

$$E(p) = \frac{\hbar u_o}{\pi a^2} (Z_1 + Z_2)^2 \int_{R_o}^{\infty} \frac{(1 - V(r))}{[1 - \frac{V(r)}{E} - \frac{p^2}{R^2}]} dR$$

$$\int_{R/2}^{\infty} \frac{\chi^2(\rho)\, d\rho}{\rho} ,$$

where u_o is the initial velocity of the ion, E is the excitation energy of the colliding particles, p is the impact parameter and V(r) is the potential of repulsion between the particles.

To obtain the correct behavior of the emission curve, the cross section of electron ejection into the conduction band had to be calculated. Because more than one electron may be lifted from the valence band to the conduction band, the cross section was determined to be

$$\sigma = \sum_{p} (\text{constant}) \cdot (\text{Probability of ionization}) \cdot (\text{Impact parameter})$$

which in the integral limit approaches

$$\sigma = 2\pi \int_0^{P_1} \frac{E(p)}{J} \, p \, dp \, .$$

Here P_1 is the impact parameter at which $E(P_1) = \delta - \phi$, where δ is the energy depth of the filled conduction band, ϕ is the work function of the target material and J is the average ionization potential for the outer shells of the atom. For $1/4 < Z_1/Z_2 < 4$ PK found the cross section to be given by

$$\sigma(u_o) = \frac{1.39 \, a_{TF} \, h}{J} \frac{(Z_1 + Z_2)^2}{(Z_1^{1/2} + Z_2^{1/2})^2} S(u_o)$$

and $S(u_o)$ is approximated by

$$S(u_o) = 5.25 \, u_o \arctan \left(.6 \times 10^{-7} \, (u_o - u_{min})\right) ,$$

where u_{min} is the threshold velocity. After determining the probability that an electron will be promoted from a filled band to the conduction band, PK assumed that most of these electrons remained in the conduction band because of the surface potential of the metal target. However, because a hole is left in the valence band, an Auger recombination is possible with subsequent emission of an electron from the metal. The probability that this process occurs is given by PK as

$$w(\delta) = 0.016 \, (\delta - 2\phi) \, .$$

PK assumed that both PSE and KSE were due to Auger processes [4].

After the secondary electrons have been produced, they suffer collisions as they proceed to the surface of the metal. These collisions degrade their energy and increase the probability that they will be lost through recombination. PK assumed that the number of electrons which reach the surface is given by an exponential law of the form exp $(-x/\lambda)$ where x is the depth at which the electrons are formed in the crystal and λ is the mean free path of the electrons in the material. Specifically, the number of electrons emitted per ion incident on the surface is given by

$$\gamma = \sum_{x} \left(\begin{array}{l}\text{Number of atoms} \\ \text{per cubic centi-} \\ \text{meter)}\end{array}\right) \cdot \left(\begin{array}{l}\text{Prob. that an electron} \\ \text{will be ejected into} \\ \text{the conduction band} \\ \text{and a hole left in} \\ \text{valence band)}\end{array}\right) \cdot \left(\begin{array}{l}\text{Prob. that an electron} \\ \text{will escape to the} \\ \text{surface of the} \\ \text{crystal)}\end{array}\right)$$

which in the limit goes to

$$\gamma = \int_{o}^{X_n} N \sigma (u) w (\delta) \exp (-x/\lambda) \, dx ,$$

where X_n is the maximum depth at which the ion retains sufficient energy to ionize a target atom. Upon taking into account the degradation of energy of the primary ion as it suffers multiple collisions and the diffusion cross

section of the electrons, PK arrived at the final expression for γ:

$$\gamma = N\, w(\delta)\, \lambda\, [\sigma(u_o) - \Delta\sigma(u_o)] ,$$

where

$$\Delta\sigma(u_o) = \exp(-u_o/(K\lambda)) \int_{u_{min}}^{U_o} \exp(u^2/(K\lambda)) \frac{d\sigma(u)\, du}{du}$$

and

$$K = \frac{2.48\pi\, N \cdot a_{TF}\, e^2\, Z_1\, Z_2}{(M_1 + M_2)(Z_1^{1/2} + Z_2^{1/2})^{2/3}}$$

The PK theory predicts the following trends [3]:

"1. Low velocity region: $u_o = u_{min}$, $\Delta\sigma(u_o)$ term is important..., γ increases slowly with u_o, $(\sigma(u_o) - \Delta\sigma(u_o)) = u_o^2 - (3/2\, u_{min})^2$. Hence initially $\gamma \propto u_o^2$, i.e., γ is a linear function of energy...

2. High velocity region: $(\sigma(u_o) - \Delta\sigma(u_o)) = u_o \tan^{-1}(.6\times10^{-7}(u_o - u_{min}))$. This expression asymptotically approaches the straight line $\sigma(u_o) = c(u_o - u_{min})$ and therefore increases linearly with velocity. Extrapolating the linear portion back to $\sigma(u_o)=0$ a value of the intercept $u_1 = 1.05\times10^7$ cm/sec is obtained; this is independent of ion target combination.

3. Very high velocities: Here ion penetration depths are greater so that electrons are formed further

from the surface. The number escaping to the surface and therefore the yield is expected to pass through a maximum. This is confirmed experimentally.

4. No yield dependence on ion charge is predicted.
5. A dependence of yield on the ion target combination of the form $((Z_1+Z_2)/(Z_1^{1/2}+Z_2^{1/2}))^2$ for heavy ions and $((Z_1^{1/2}+Z_2^{1/2})(Z_1^{1/6}+Z_2^{1/6})^3)$ for light ions. If the term $\Delta\sigma(u_o)$ is important...the yield is independent of ion-target combination to a first approximation.
6. Dependence of yield on the angle of incidence θ is expected to be of the form $\gamma_i = \sec\theta$ since the probability of electron escape is a function of the shortest distance to the surface and the probability of formation of electrons is a function of the actual distance traversed.
7. The effect of the isotopic mass on yield is anticipated to be connected with the different retardation rates for the isotopic pairs." [3]

All of these conclusions are approximately confirmed by the experimental results.

B. THE THEORY OF HARRISON, CARLSTON AND MAGNUSON

The PK theory uses many simplifying assumptions which introduce approximations into the results obtained. In

particular, the PK theory predicts secondary electrons of only average energy, two to five ev, and data obtained by Wolff [6] of SEE from copper bombarded by ten Kev argon ions indicates some secondary electrons emitted have energies greater than 140 ev.

In the PK theory secondary electron emission was viewed as a two-step process in which ions were first produced along a path in the target material and subsequently diffused to the surface with possible scattering or Auger emission occurring along the path. This model does not yield the high-energy secondary electrons which are reported experimentally. In an effort to explain this discrepancy between experimental and theoretical result, Harrison, Carlston and Magnuson [2] (HCM) proposed a "single collision" theory of secondary emission. This theory, though in many respects similar to the PK theory, has as its basic philosophy an electron production mechanism which differs from the model proposed above.

HCM proposed a model in which an ion approaching a target surface first undergoes resonance neutralization and subsequently collides with the first layer of atoms in the target material in the un-ionized state. Even though the primary particle is neutralized before the collision, the terminology of "ion" is retained here to distinguish between the primary particle and the target atom after collision. For simplicity HCM assumed that the electrons liberated due to the inelastic energy transferred between the electronic structures of the

ion and the atom all come from the ion, which allowed them to ignore the energy partition between collision partners. Theoretical work by Harrower [7] indicates that the Auger process requires a time on the order of 10^{-14} seconds while in the one to ten Kev energy range the collision process takes on the order of 5×10^{-14} seconds. This indicates that, statistically, the ion usually does not have time to neutralize before its next collision and for all practical purposes cannot contribute further to the secondary electron emission process. These results lend credence to the single collision model. Mathematically HCM proposed:

$$\gamma_{KSE}^{(hk\ell)} = K \int_{o}^{s_{MAX}^{(hk\ell)}} n_e\,(s, E_{TFF})\; P^{(hk\ell)}\,(s)\; ds\;,$$

where $\gamma_{KSE}^{(hk\ell)}$ is the number of electrons emitted per incident ion when the ions are normally incident upon the (hkℓ) surface; s is the impact parameter of the ion on the atom; E_{TFF} is the inelastic energy transfer between the ion and the atom; $n_e^{(hk\ell)}(s, E_{TFF})$ is the number of electrons this energy will produce; and $P^{(hk\ell)}(s)$ is the probability that the impact parameter s will occur in the (hkℓ) surface. This equation contains three adjustable parameters, the constant K and two constants which enter into the calculation of ϕ, the electron density, and the interaction potential V(r). By symmetry, these last two constants must be the same for all orientations of the particular crystal plane, (hkℓ), in question.

According to HCM, the constant K is a factor which accounts for three physical processes:

1. The probability that an electron will be emitted from the surface (a value close to 1/2);
2. The probability of additional emission by an Auger process; and
3. The probability that a high energy electron escapes before it is scattered back into a conduction band. [2]

All of these processes are orientation independent. The factors which appear in the formulation of the HCM secondary electron emission equation are discussed in detail below.

1. The Inelastic Energy Transfer

In the HCM theory E_{TFF} is the inelastic energy transferred in the collision process and is basically the same as E(p) in the PK theory. However, as HCM point out, because the interaction involves atoms spaced regularly in a lattice array, the inelastic energy integral does not have an infinite upper limit as was assumed by PK. Specifically,

$$E_{TFF}(s,E_o) = K_{TFF} \int_{r_{min}}^{r_{max}} \frac{(1-V(r)/E_o)\, dr}{(1-V(r)/E_o - s^2/r^2)^{1/2}} \cdot \int_{r/2}^{r_{EM}} \phi^2 \frac{(\rho)\, d\rho}{\rho}$$

where

$$K_{TFF} = \frac{h}{\pi a_H^2} (E_o/(2m_1))^{1/2} (Z_1+Z_2)^2 \quad ,$$

$$a_H = h^2/(me^2) = .529 \text{ Å}$$

and E_o is the energy of the ion in the center of mass system; Z_1 and Z_2 are the ion and atom nuclear charges, respectively; r_{min} is the distance of closest approach; and ϕ is the Thomas-Fermi (TF) screening function:

$$\phi(\rho) = [1 + (a_F\rho)^{0.8034}]^{-3.734}$$

where

$$a_F = \frac{a_{TF}((Z_1+Z_2)/144)^{1/3}}{0.8853}$$

and a_{TF} is one of the adjustable constants introduced above. By experimenting with different sets of potentials, in conjunction with the screened electron distribution, HCM found that the best agreement with experiment was obtained when the potential V(r) was of the Born-Mayer form [2]:

$$V(r) = \exp(A+Br) = A' \exp(Br)$$

with B always negative, and where A is the second of the above mentioned arbitrary constants. HCM referred to the integral containing $d\rho$ as the electron integral. The convention is retained here.

Several important results were noted by HCM in the formulation of their original model. First, the dynamical integral was extremely sensitive to its upper limit $r_{max}^{(s)}$, whereas the electron integral was not sensitive to variations in r_{EM}. For this reason r_{EM} was set at a value somewhat larger than the nearest neighbor distance R_o, in the crystal lattice, and retained this value for all orientations of the crystal lattice. On the other hand, the upper limit of the dynamical integral was extremely sensitive to the nearest neighbor distance. Such a behavior is expected because as each ion collision with a particular atom terminates, another must begin with one of its neighbors. From a particle dynamics point of view, HCM found that by treating the actual collision with the lattice as a binary collision between the incoming ion and any single atom within the first repeat distance of the crystal plane, the theory yielded results which approximated those obtained by experiment. Figure 3 indicates the geometrical relationship between various quantities associated with the dynamical integral [2].

2. Collision Parameters

Because of the repetitive nature of the lattice, or lattice plane, it is not unreasonable to think of a "representative area" which characterizes the lattice plane as a whole and hence its distribution of impact parameters. If no lattice were present, and only one target atom, there would be no characteristic area and the occurrence of a

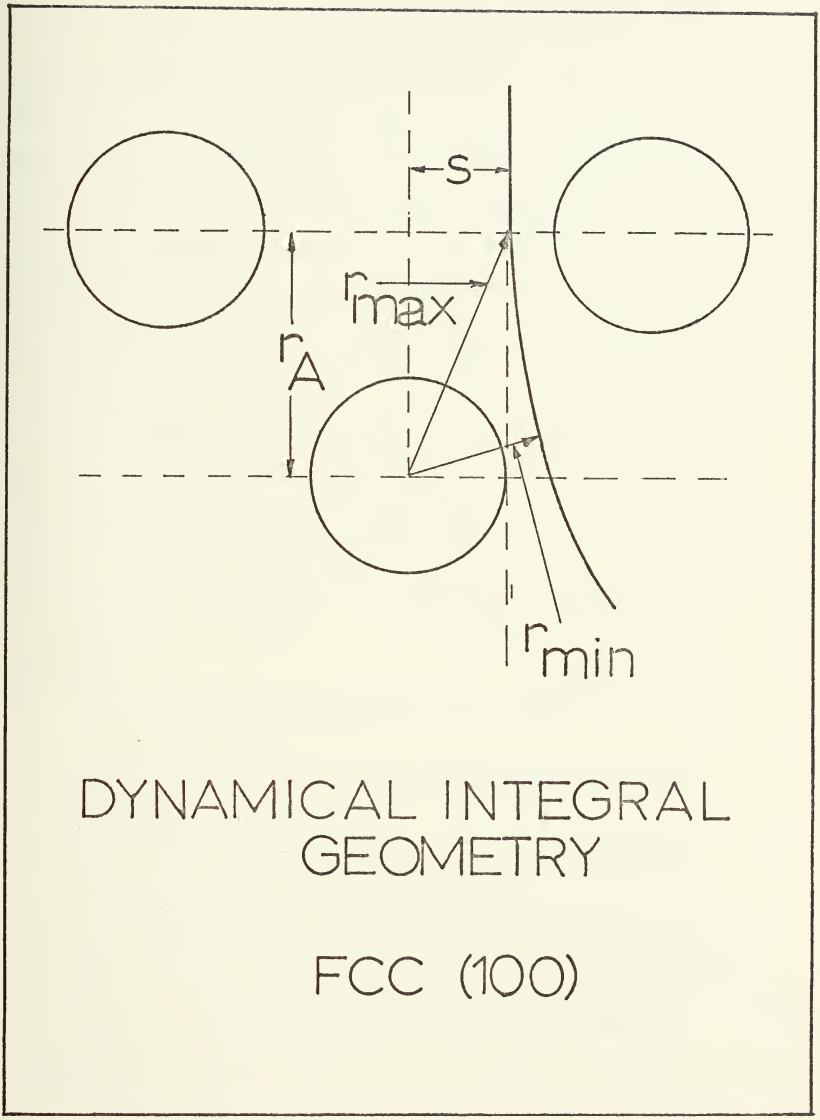

Figure 3. Relationships between various quantities appearing in the Dynamical Integral.

collision with any impact parameter would be possible, yielding an infinite collision cross section. As an ion approaches a plane of atoms in a crystal, however, there exists an allowable set of impact parameters for the ion-atom collision. Specifically, in a lattice there exists an impact probability distribution, $p^{(hk\ell)}(s)$, for each crystal orientation. For normal incidence HCM proposed the areas shown in Figure 4. These areas are representative of the normal impact of an ion with any atom on the specified crystal surface, viz., by symmetry operations they fill plane space and are representative under any of these symmetry operations of what an ion "sees" as it approaches the planar surface normally. There are many distributions which could be considered probability distributions. HCM considered the following:

1. The distribution of values of s measured to the nearest surface atom;
2. The distribution of all values measured to all atoms which project their area into the representative area;
3. The distribution of smallest impact parameters when all atoms are considered [2].

The third case was the only one which yielded results in agreement with the experimental data. The distributions for normal incidence on FCC and BCC metal targets are shown in Figures 5 and 6.

Operationally, the distributions are determined as follows: First, the representative area is chosen. "Points" are shot at the representative area, and the distances

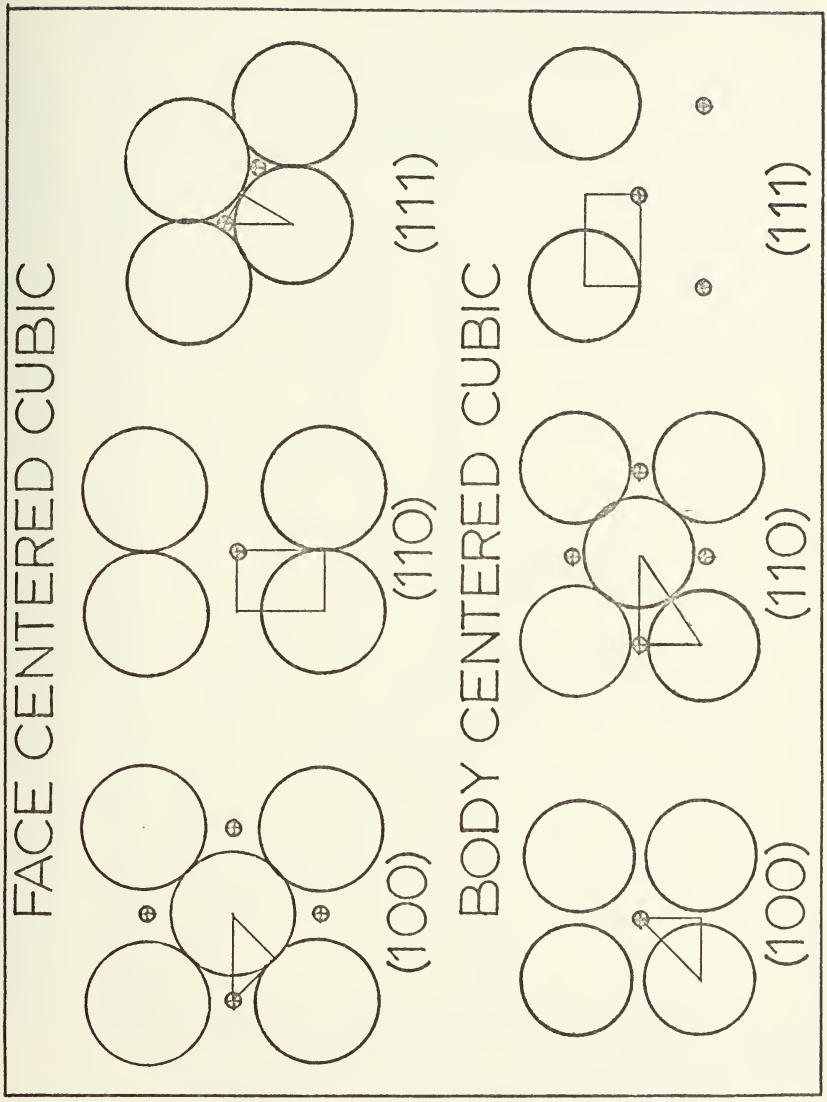

Figure 4. Representative areas for normal incidence. After (2).

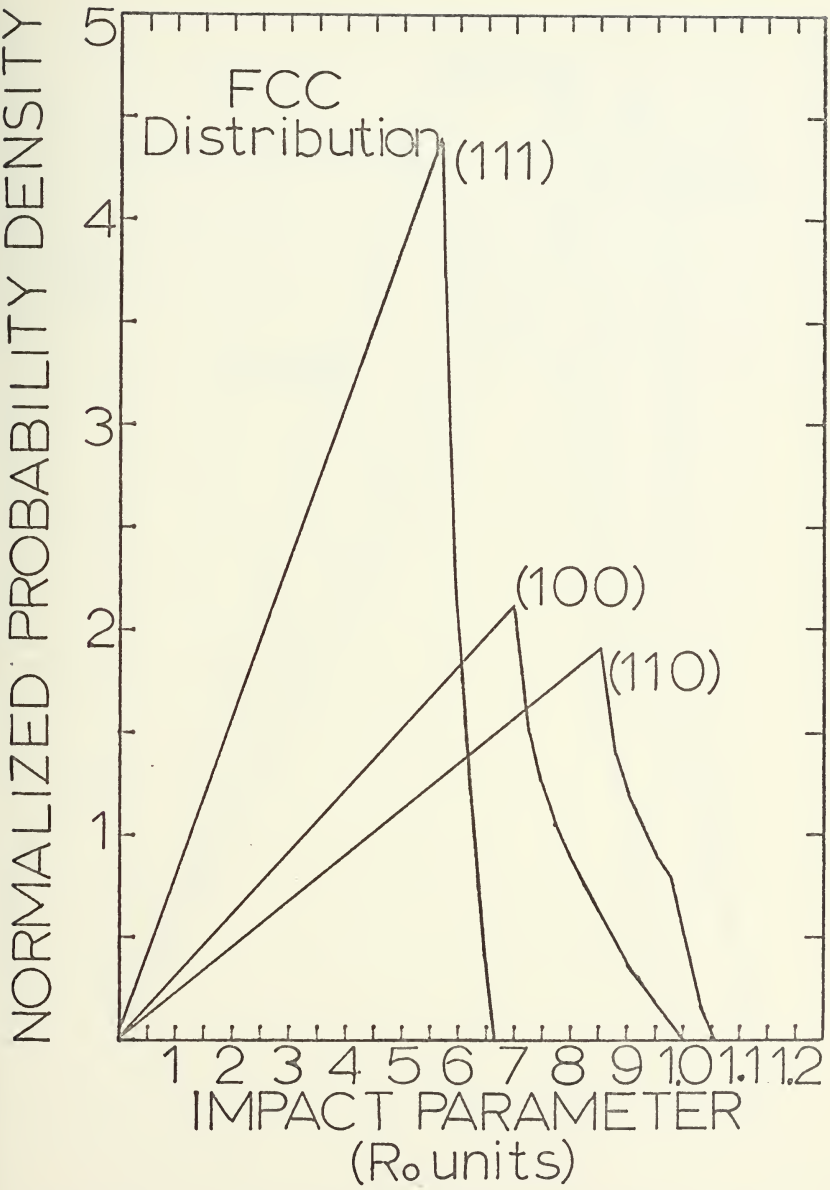

Figure 5. Distribution of impact parameters for normal incidence on face-centered cubic crystals.

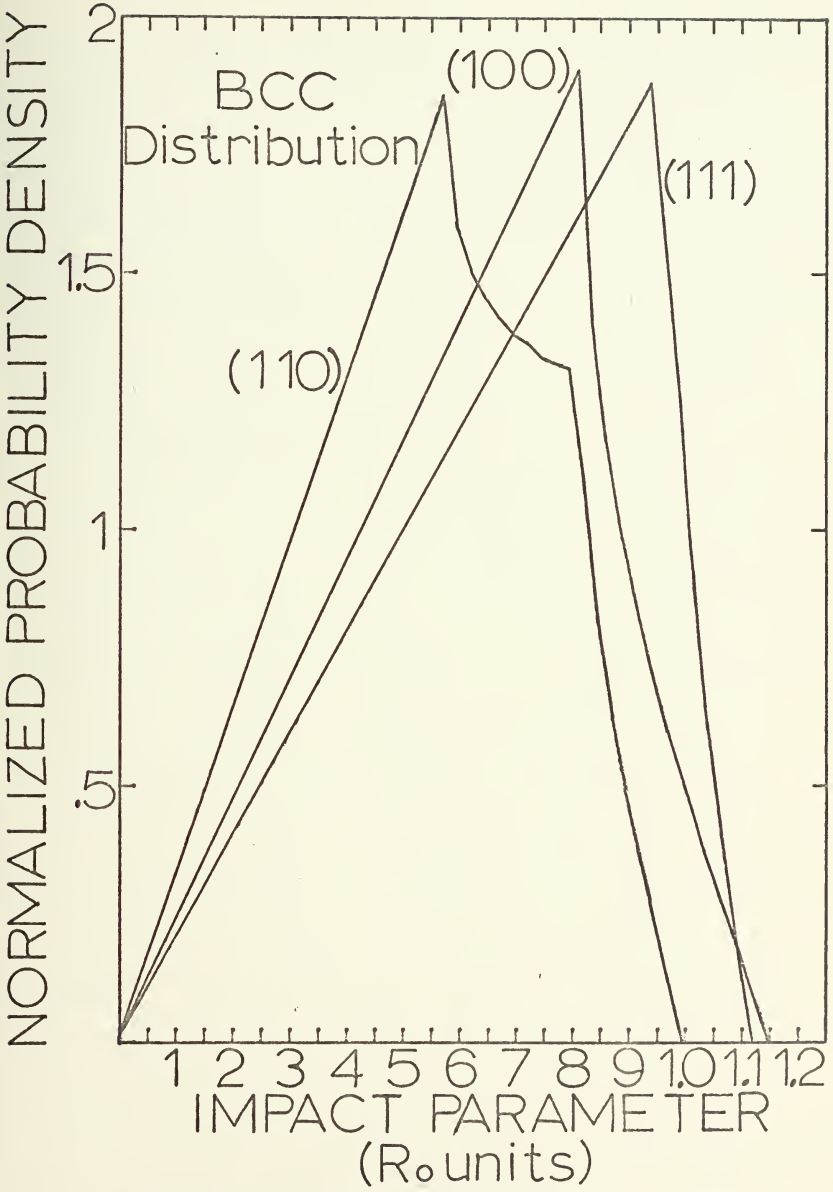

Figure 6. Distribution of impact parameters for normal incidence on body-centered cubic crystals.

between the impact point and the centers of the atoms lying in the representative area are measured. For each atom the distances for points that are measured to be closest to it are tallied. After a sufficient number of points are tallied to yield good statistics, the distribution for each atom is weighted by a factor to account for the fractional portion of atom lying in the representative area. The atoms' distributions are then added and scaled so that the total area under the resulting curve is unity.

3. Number of Electrons Emitted--Russek Model

One of the major shortcomings of the PK theory was that it used average ionization energies to obtain an ionization cross section. This is to say the PK theory did not consider the electronic structure of the target atom. HCM adopted a model proposed by Russek [9] to obtain the number of electrons liberated per collision, $n_e^{(hk\ell)}(s,E_{TFF})$. In his original paper, Russek proposed two ionization models of interest, the uniform ionization model (UI), and the staggered ionization model (SI). The UI model assumed that as electrons were liberated by the collision process, the amount of energy required to liberate any one electron was the same as that required to liberate any other electron. On the other hand, the SI model assumed that each electron liberated required more energy than was required to liberate the preceding electron. For the SI case Russek shows that the probability that n electrons will be liberated from a shell, which contains M electrons is given by:

$$P_n^{(M)} \sim \binom{M}{n} \sum_{i=0}^{k} (-1)^i \binom{M-n}{i} \left(\frac{1 - nE_n^{ION} + iE_{n+1}^{ION}}{E_{TFF}}\right)^{M-1}$$

where $k \leq (E_{TFF}/E_{n+1}^{ION} - nE_{n+1}^{ION}/E_{n+1}^{ION}) \leq k+1$ and M is the number of electrons available in the outermost shell of the atom; E_n^{ION} is the energy required to remove the n^{th} of these electrons and E_{TFF} is the energy available to cause this removal. Two things should be noted. First, the impact parameter enters this calculation through the inelastic energy transfer. Second, when $E_{n+1}^{ION} = E_n^{ION}$ one obtains the UI model. After normalizing the function, $P_n^{(M)}$, viz.,

$$\sum_{n=0}^{N} P_n^{(M)} = 1$$

then, from probability arguments, the number of electrons liberated is:

$$\overline{n_e(E_{TFF})} = \sum_{n=0}^{M} P_n^{(M)} n_e \ .$$

HCM were unable to obtain good results with the Russek UI model. In all cases, γ increased much too rapidly as a function of energy. On the other hand, the SI model yielded reasonably good results, where spectroscopic values for E_n^{ION} were used.

4. HCM Results

HCM investigated the Ar - Cu system in detail. They first examined the E_{TFF} dynamical integral for various types of potential functions and found that the PK potential which was of the Thomas-Fermi-Firsov type was too hard for small values of E_o, viz., the hard core radius of the target atom was too large, in this energy range, to yield acceptable results. Attempts at softening the potential by decreasing a_{TF} failed. For this reason HCM assumed a potential function of the Born-Mayer type. The potential function used in each case was found by matching the exponential to the TF screening function at some separation.

HCM assumed that the experimental data contained both potential, γ_{PSE}, and kinetic, γ_{KSE}, contributions to the total secondary electron emission coefficient. Therefore, HCM identified the γ at which KSE begins to contribute as γ_{PSE} and assumed this value remains constant for all energies. This value for γ_{PSE} was then subtracted from the experimentally determined γ for the (111) surface at 10 Kev. The (111) value of γ_{KSE} at 10 Kev, obtained from theory, was scaled to this point, and all other points were multiplied by the scale factor used in performing this operation. Finally the constant value of γ_{PSE} was added to all the scaled theoretical values. The result is the HCM value for the total secondary electron emission. The results of the HCM theory for the Ar^+ - Cu system are presented in Figure 7.

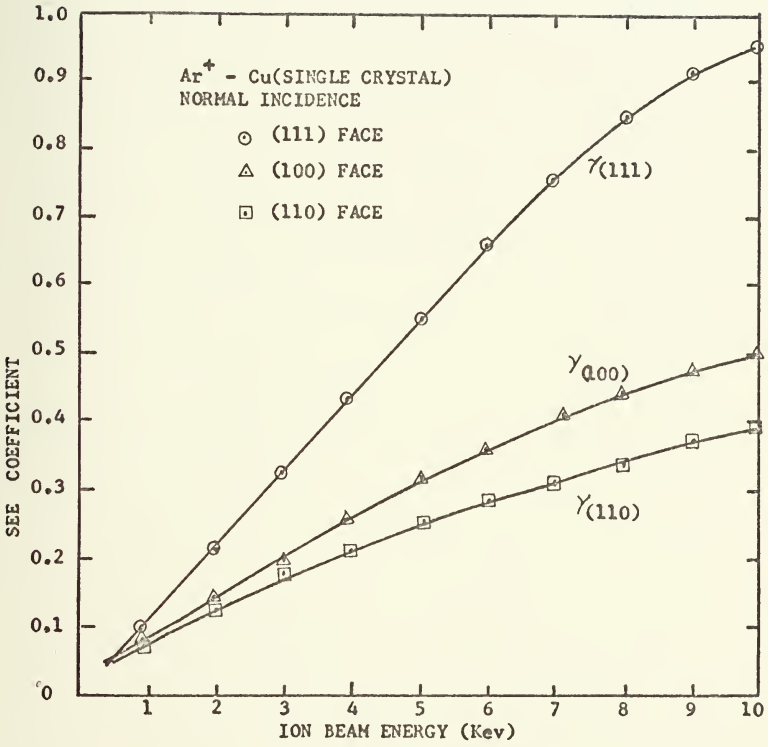

Figure 7. Ar^+ - Cu results obtained from the HCM original model. Taken from (2).

In general, HCM's theory agrees reasonably well with experimental results for all systems studied except Ar - Mo.

V. MODIFICATIONS TO THE HCM THEORETICAL MODEL

A. INTERATOMIC POTENTIAL

Independent of the philosophy behind the basic interaction, the HCM theory, like the PK theory, is highly dependent on two specific assumptions. First, both assume that the inelastic energy transferred is of the form proposed by Firsov. Second, both theories must assume an interatomic potential function which is consistent with the electron distributions of the ion and atom. Since the Firsov model is presently the only comprehensive model available for the inelastic energy transfer, it has been retained here as an approximate model of the inelastic collision process and is assumed to be sufficiently accurate for our purposes. However, the interaction potential used in the Firsov model need not be of the Thomas-Fermi form, but may be derived from a more accurate representation of the electron distributions of the ion and atom.

The interaction potential is derived from the electron distributions of the collision partners. These potentials exist on three general levels of sophistication: (1) The Bohr and Born-Mayer potentials which are derived from electron distributions which provide screening of the nucleus in a self-consistent, but not necessarily accurate, manner; (2) Thomas-Fermi and Thomas-Fermi-Dirac potentials which are derived from statistical pictures of the electron

distributions of the collision partners; and
(3) Potentials generated from electron densities derived numerically from Schroedinger's equation.

Parilis and Kishinevskii used a Thomas-Fermi potential function in the theory they proposed. Statistical models of the atomic electron distribution, such as in the TF model, are based on studies of inhomogeneous gases and approximate solutions of Schroedinger's equation consistent with this picture [10, 11]. They require that the total electron energy be a minimum and that the electron density integrate to the total number of electrons in the system. Approximations may be made to evaluate the exchange and correlation energies. When the exchange and correlation energies are omitted and the kinetic energy is approximated by a plane wave, the TF atomic model results [11]. If the exchange energy is retained and the kinetic energy is approximated by a plane wave, the TFD atomic model results [11]. The TF model of the atom has been used extensively by Firsov, whereas the TFD model appears in papers by Abrahmson [13].

Potential functions based on Hartree-Fock solutions of the atomic Schroedinger equation have been discussed by Wedepohl [12], Harrison [13], and Wilson [14]. These potentials assume the adiabatic approximation, use spherically symmetric electron distributions which have shell structure, and take into account the correlation,

kinetic and exchange energies through various approximations. They appear to lead to improved calculations of the interaction potential [8, 14, 15]. The present investigation utilizes an interaction energy calculation similar to that proposed by Wedepohl [12]. However, the electron densities from which the potential is derived are calculated from the Hartree-Fock-Slater self-consistent wave functions calculated from the Herman-Skillman [16] computer program. The reader is referred to the original book [16] for detailed information on the calculation of the atomic electron distribution functions and to the work by Torrens [8] for a general discussion of the interaction potential.

B. THE BASIC INTERACTION

Harrison, Carlston and Magnuson assumed that all of the secondary electrons produced in the single collision model came from the ion. This assumption was tested by choosing various values of E_n^{ION} in the Russek model and noting the dependence of $n_e(E_{TFF})$ on E_1^{ION}. This experiment was carried out for the Ar^+ - Cu system. The results were most favorable for E_1^{ION} equal to 15.8 ev, the first ionization potention of argon, and least favorable for neutral copper's first ionization potential. This approximation was an attempt to simplify the model so that detailed models of energy sharing mechanisms could be avoided. In this present investigation, this assumption has been relaxed to include contributions to the secondary emission by the target atom.

Theoretically, the interaction is viewed as the collision of two atoms having spherically-symmetric, shell structured electron distributions. As the atoms collide, they are assumed to form a "molecular" structure whose electron ionization potential distribution is comprised of the separate ionization potentials of the electrons of the atoms involved in the collision. Since electrons are ejected on a "least energy" principle, the values of E_n^{ION} used in the Russek model have been modified by include both primary ion and target atom ionization energies which are arranged in increasing order of magnitude, irrespective of the atom to which they belong. The mean number of electrons is a complicated function of the inelastic energy transfer and the energy necessary to effect each electron's removal.

C. THE DISTRIBUTION OF IMPACT PARAMETERS

To accomplish the objectives of this present investigation, one additional modification to HCM's original paper had to be made. Since the angular dependence of γ was to be studied, a new distribution of impact parameters had to be calculated. Fortunately, according to the HCM paper, this modification to the mathematical model is the only change required to take into account rotations of the crystal plane around an arbitrary crystallographic direction. No other factor entering into the secondary electron emission equation is orientation dependent [2].

Two possible solutions to this problem are proposed below. First, a crystal plane normal to the direction of incidence of the ion beam can be found, from which a representative area can be constructed. Such a formulation would be analogous to cutting the crystal in such a manner that it presented a planar area normal to the incident ion beam and finding an area on this plane which would be representative of that orientation. Alternatively, a representative area constructed from the crystal face which was experimentally rotated can be used and mathematically rotated about the specified crystallographic axis. In practice, the first method is computationally restrictive because it requires that a representative area on a plane normal to the incident ion beam be found for each orientation. For this reason it is not pursued further here.

The second method mentioned above yields a result that is more in line with the reasoning behind HCM's original definition of the distribution of impact parameters. Practically speaking, a representative area is found for each crystal face which fills plane space and is representative of what an ion sees as it approaches the crystal plane from an arbitrary direction. Unlike the representative areas for normal incidence, angularly dependent representative areas must be truly representative for all possible rotations of the plane and not simply for one particular orientation. The representative area for the FCC (100) surface which can be rotated in either a positive or negative

sense about the <$\bar{1}$10> crystallographic axis is shown in Figure 8. Note that atoms which lie within the first repeat distance of the crystal plane are eligible target atoms in the representative area by HCM's definition of representative area. Also note that these atoms from the lower atomic plane appear to move as the crystal plane is rotated in a positive sense about the <$\bar{1}$10> axis (see Figure 9). This behavior can be verified by physically rotating a stick and ball model of the lattice structure about the indicated axis.

Once the representative area is chosen, its rotational properties and corresponding distribution of impact parameters are calculated as follows. The representative area is placed in the first quadrant of a rectangular coordinate system (x,y) (see Figure 10). In this system, the crystallographic axis of rotation is specified by two parameters:

1. The angle of the crystallographic axis makes with the x-axis of the rectangular coordinate system (x,y); and
2. The y-axis intercept of the crystallographic axis in the rectangular coordinate system (x,y).

This system of coordinates is then transformed into a primed rectangular reference frame (x',y') for which the crystallographic axis of rotation is the x'-axis, and whose origin is the point at which the crystallographic axis intercepts the y-axis, (x_R, y_R) (see Figure 10). The equations relating the transformation of points from the (x,y) coordinate

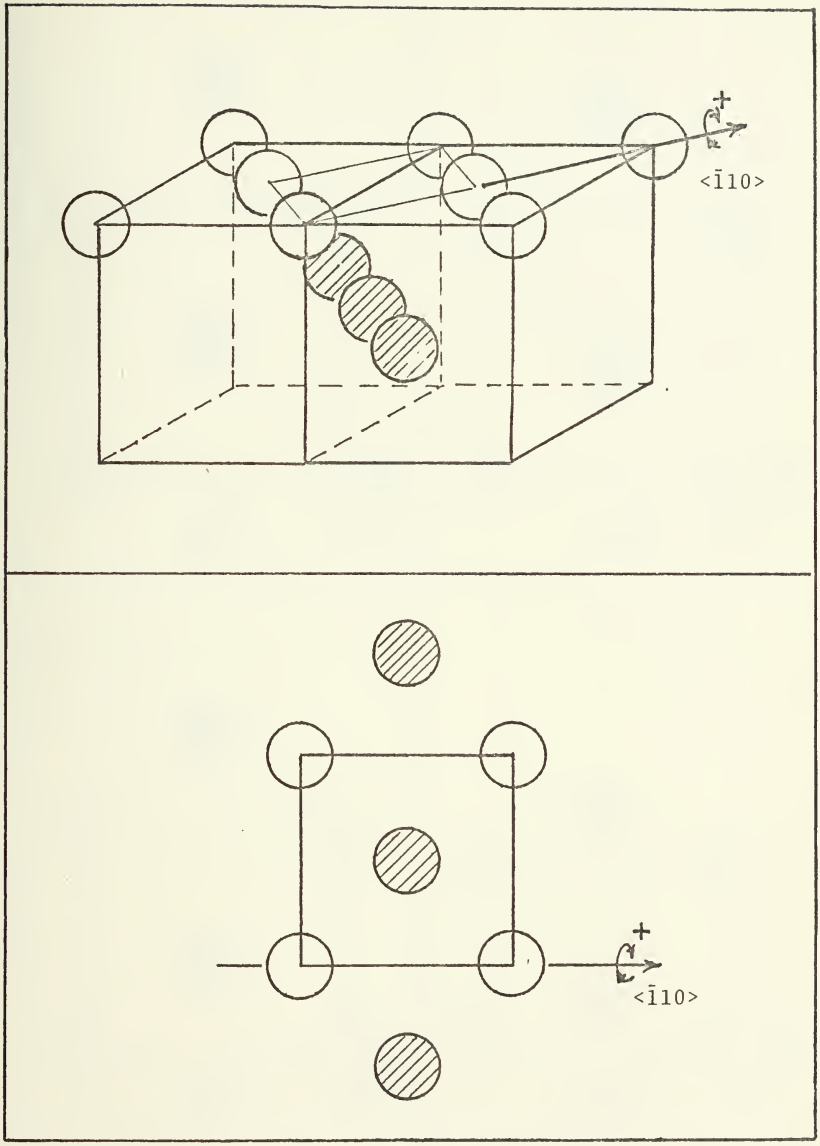

Figure 8. Representative area of a (100) FCC crystal face rotated about <$\bar{1}$10> in either a positive or negative sense.

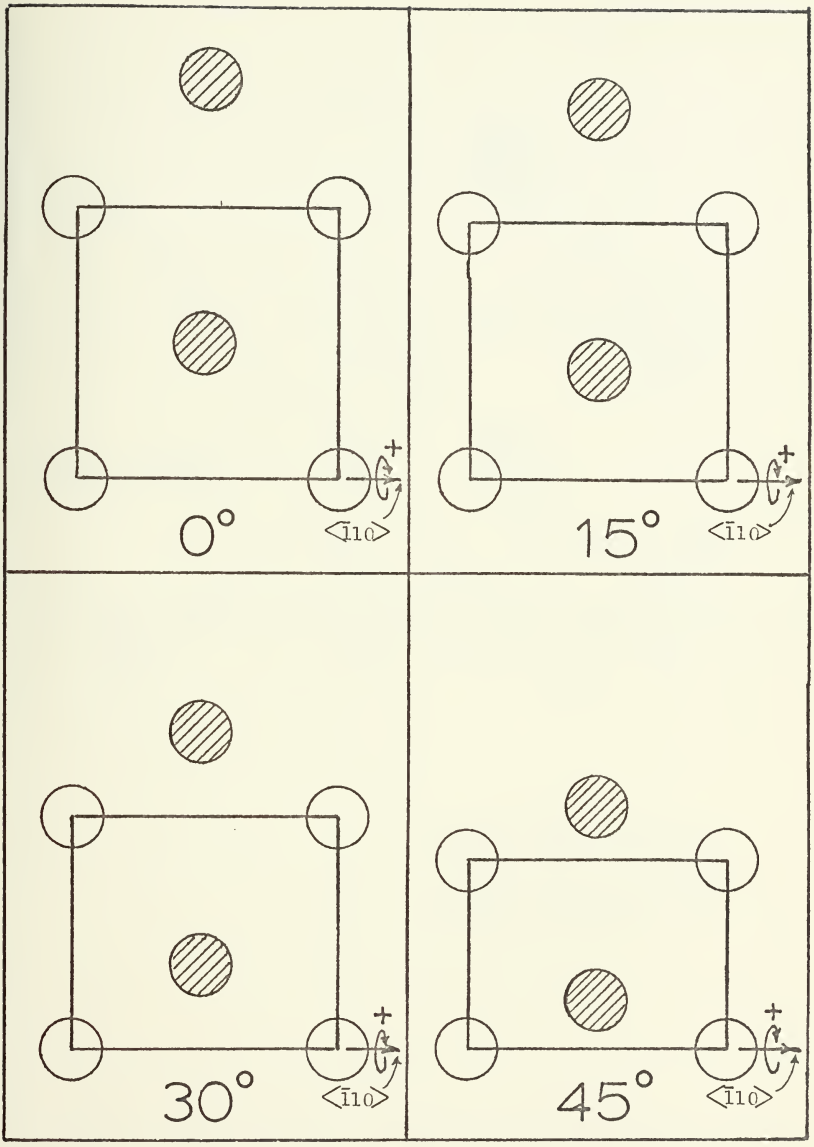

Figure 9. Representative area of the (100) face of an FCC crystal rotated in a positive sense about the <1̄10> direction.

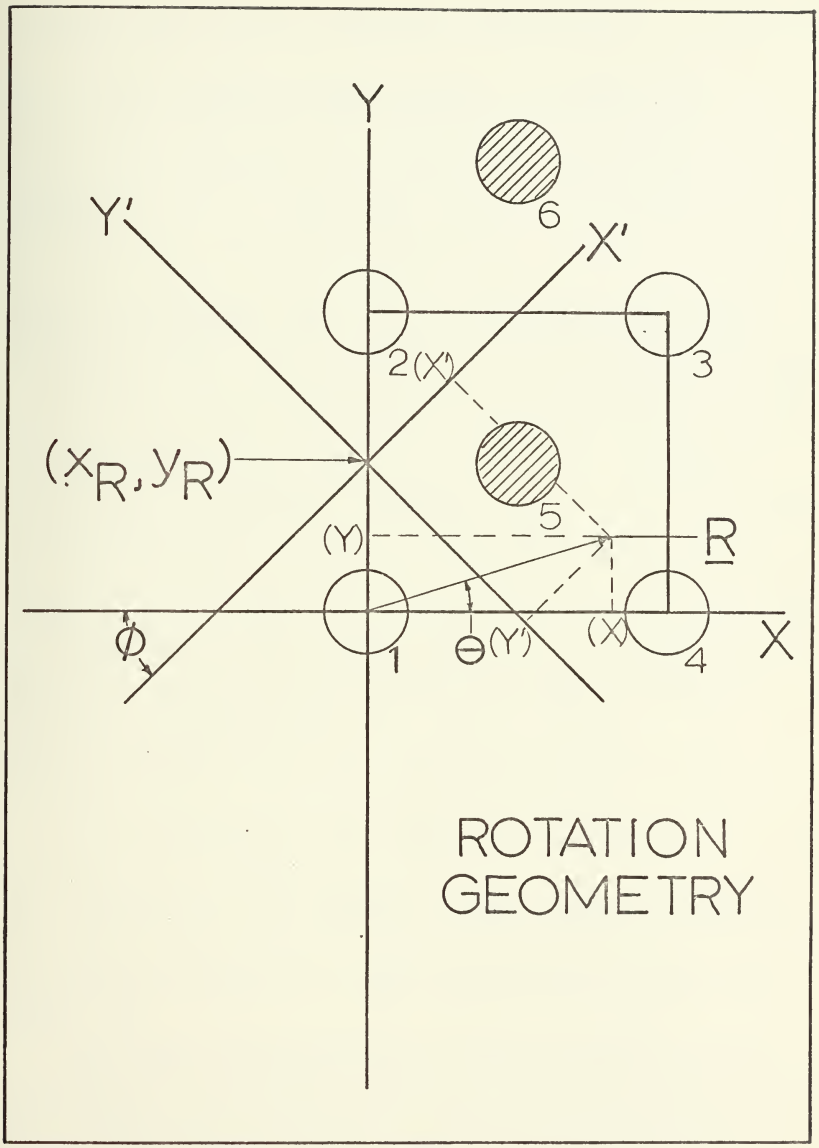

Figure 10. Rotation geometry for a (100) face of an FCC crystal about an arbitrary crystallographic direction.

system to the (x',y') coordinate system are:

$$x' = R \cos(\theta - \phi) - (y_R \sin\phi + x_R \cos\phi),$$

$$y' = R \sin(\theta - \phi) + (x_R \sin\phi - y_R \cos\phi).$$

where

$$R = (x^2 + y^2)^{1/2}$$

$$\theta = \arctan(y/x)$$

and ϕ is the angle that the crystallographic axis makes with the x-axis. If the system is rotated through an angle α about the x'-axis, distances to any point (x',y') appear to be shortened by an amount cos α in the y' dimension, leaving the x' dimension unchanged. Also, if the atom whose projected position lies at (x',y') before rotation is an atom whose actual position is R_a units below the plane being rotated, then its new apparent position on a plane perpendicular to the direction of incidence after rotation is given by the doordinates $(x', y' \cos\alpha - R_a \sin\alpha)$. In general then the final transformation equations become:

$$x' = R \cos(\theta - \phi) - (y_R \sin\phi + x_R \cos\phi),$$

$$y' = (R \sin(\theta - \phi) + (x_R \sin\phi - y_R \cos\phi)) \cos\alpha - R_a \sin\alpha .$$

The geometry implicit in these calculations is shown in Figure 10.

The actual calculation of the distribution of impact parameters is performed as follows. A mathematically constructed, rectangular grid is placed over the area and points which lie within the representative area are

systematically chosen. Using the transformation equations and the known position of the atoms in the representative area, the distance from the points chosen in the area to each respective atom are calculated in (x',y') coordinates and the shortest distance is chosen. The shortest impact parameter is tallied against the atom with which it is associated, in an array. In the case of equal distances between two atoms, the atom with which the ion impacts is chosen by a uniformly distributed pseudorandom process [17]. The final array contains the distribution of all impact parameters tallied with each atom in the representative area. To obtain the final distribution of impact parameters for the crystal face, the individual distributions are weighted, added, and the area under the curve is normalized to unity. The number of points used in calculating these distributions are on the order of 100,000 per representative area. The final unnormalized distribution of impact parameters for (100) FCC crystals for various angles of rotation is shown in Figure 11. Note that all dimensions used in calculating these distributions are in terms of R_o, the nearest neighbor distance in the crystal lattice.

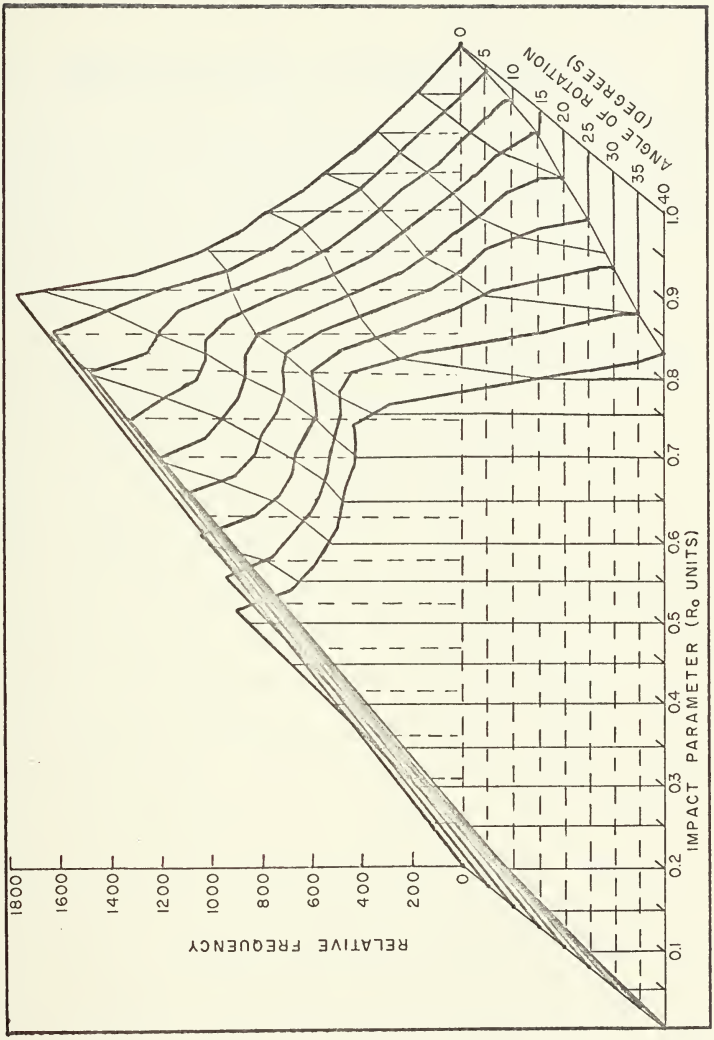

Figure 11. Unnormalized distribution of impact parameters for FCC (100) rotated through various angles about <$1\bar{1}0$>.

VI. NUMERICAL METHODS AND COMPUTER PROGRAMS

The theory presented in the preceding chapters has been incorporated into five FORTRAN IV computer programs which are presented in the appendix to this thesis. They appear in the order of their use. Specifically, these programs are:

1. The Herman-Skillman radial-electron density program,
2. The Harrison potential program,
3. Distribution of impact parameters program,
4. Numerical interpolation program, and
5. The Harrison KSE program.

To calculate the coefficient of ion-electron emission (SEE coefficient), these programs are utilized in the following manner. The ion-atom-radial-electron densities are calculated using the Herman-Skillman computer program [16]. These densities are put into the Harrison potential program which calculates the interatomic potential, V(r), used in the calculation of the inelastic energy transfer, E_{TFF}. The distribution of impact parameters program calculates the distribution of impact parameters for each crystal face under investigation. Since this is a statistical process, the distributions recovered from this program are "smoothed" using a first and tenth degree Legendre orthogonal least squares interpolating polynomial, which is generated by the numerical interpolation program [18]. Finally the

smoothed distribution of impact parameters and potential function are inserted into the Harrison KSE program which has been modified to include all the changes to the original theory presented in the "Modifications" chapter of this thesis. This program performs the actual calculation of the SEE coefficient using the HCM model. The input data format to each of these programs is shown in Figures 12 through 16. The definitions of the input variables used in the programs are presented in Appendix A to this thesis. The results presented in the following chapter were run on the Naval Postgraduate School IBM/360 Computer System.

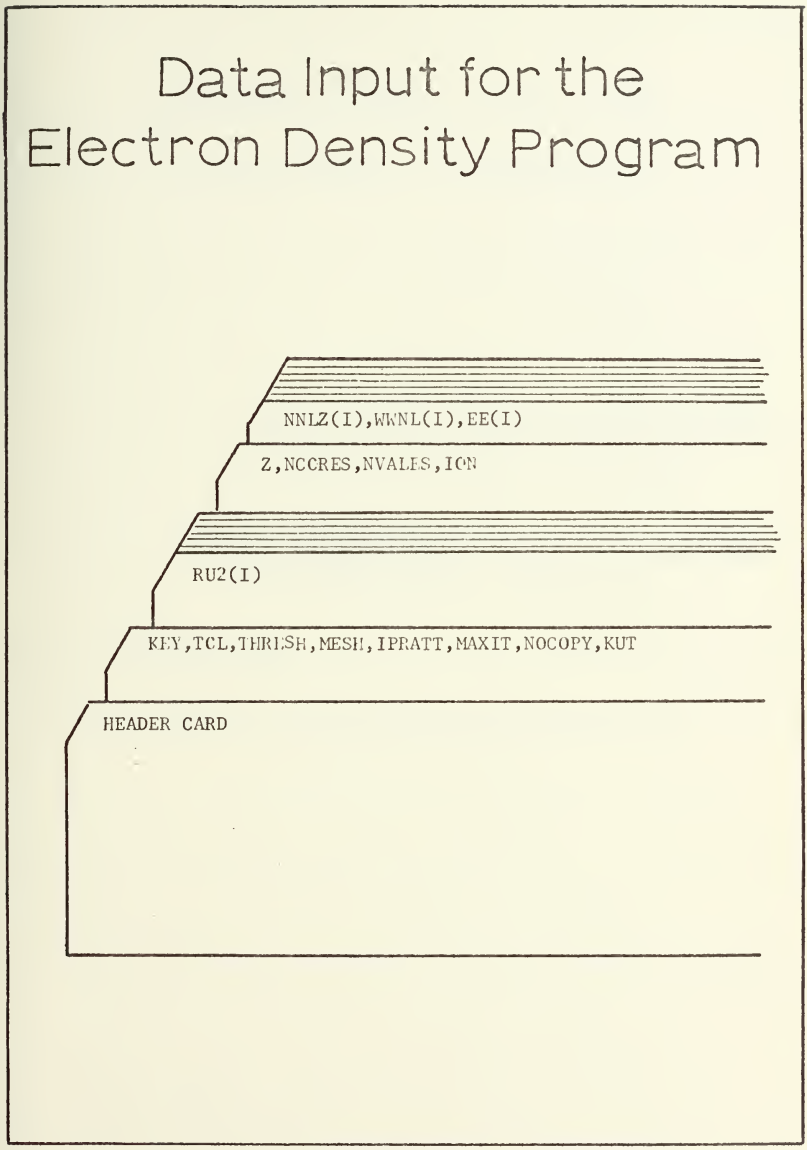

Figure 12. Deck setup for running the Electron Density Program.

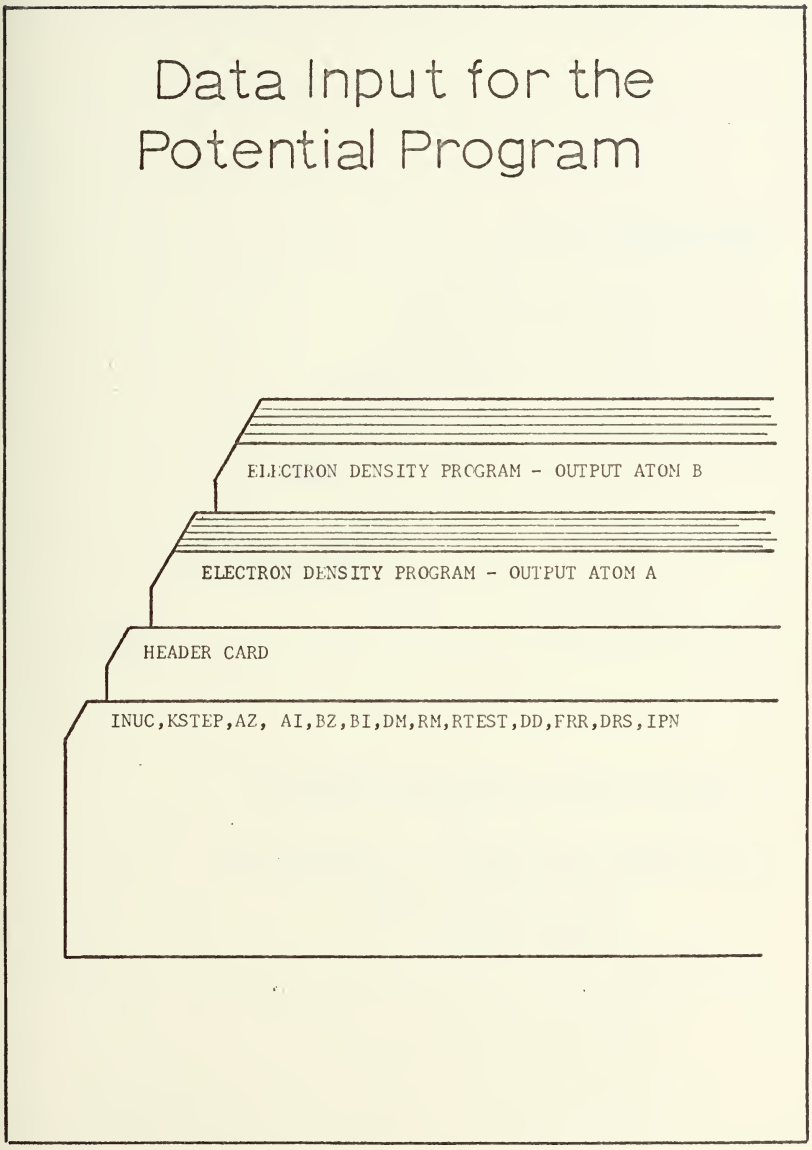

Figure 13. Deck setup for running the Potential Program.

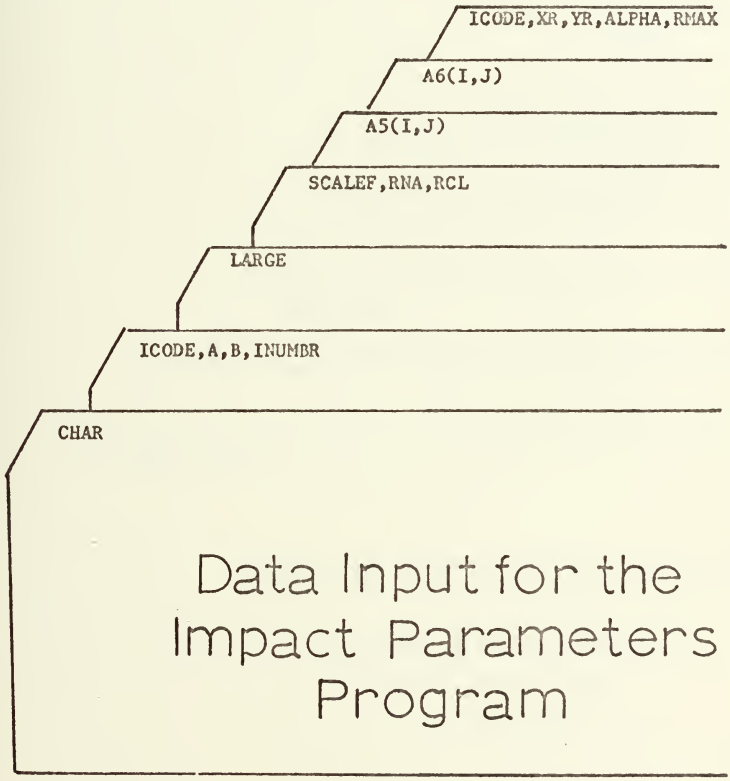

Figure 14. Deck setup for running the Distribution of Impact Parameters Program.

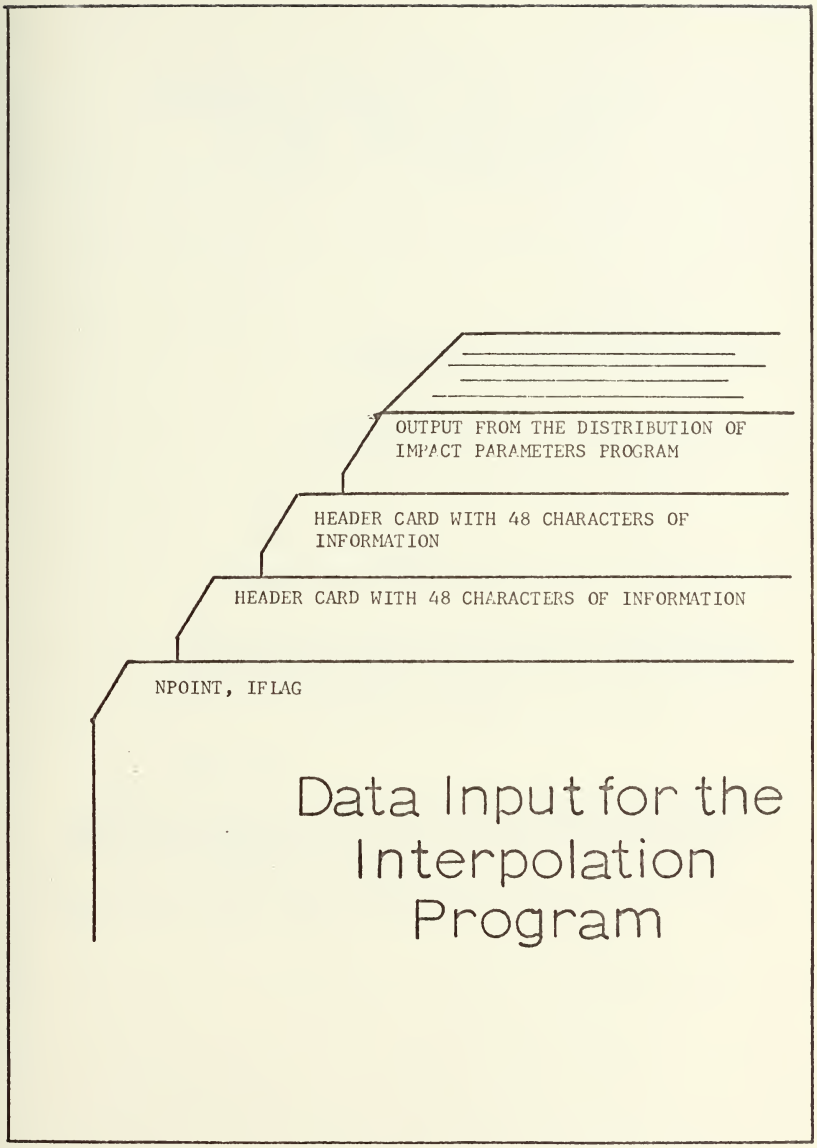

Figure 15. Deck setup for running the Interpolation Program.

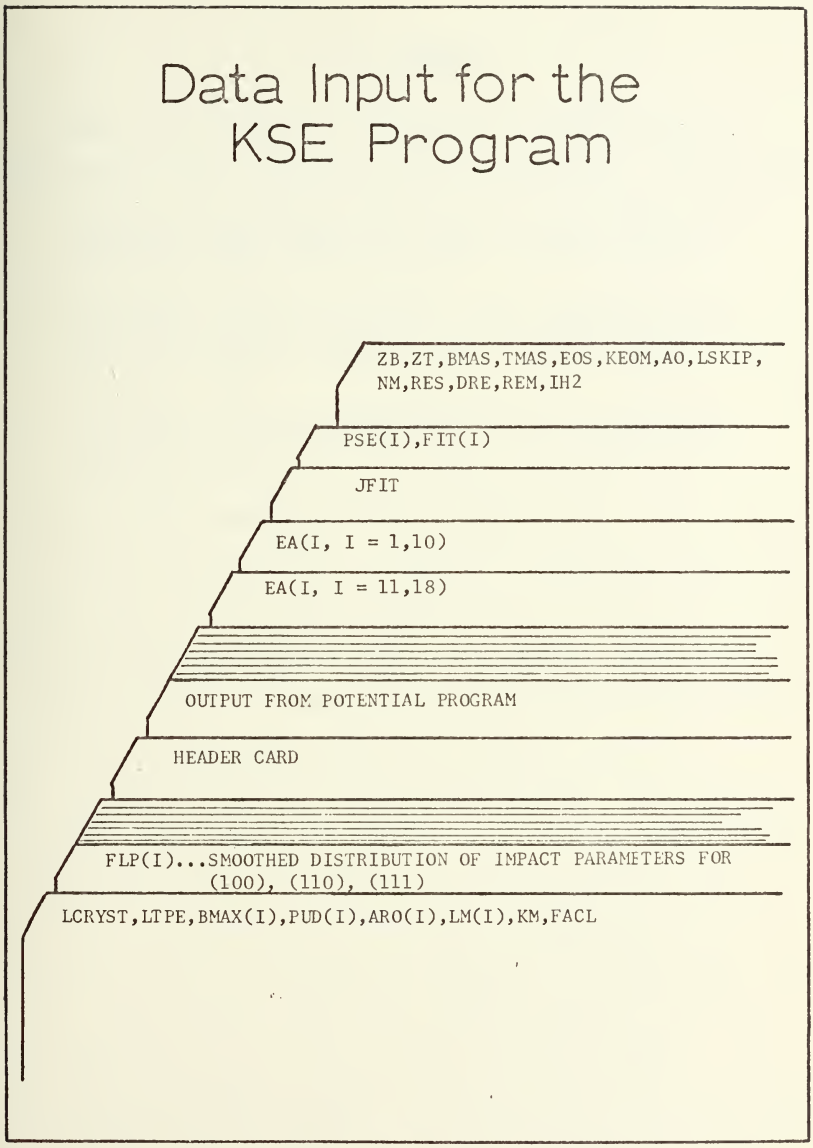

Figure 16. Deck setup for running the KSE Program.

VII. RESULTS

Three separate cases of secondary electron emission were investigated using the modified HCM model. These were:

1. Angularly dependent secondary electron emission from the (100) face of a copper single crystal rotated about a <$\bar{1}$10> axis;

2. Secondary electron emission from Ar, Ne, Kr and Xe ions normally incident on the (100), (110) and (111) faces of Cu, Ag, Mo, and Al single crystals; and

3. Secondary electron emission from Ar and Ne ions normally incident on the (100), (110) and (111) faces of KCl.

In the HCM theoretical model, the primary ion is assumed to be neutralized before it strikes the target surface. The target atoms in the metal are assumed to be ion cores in a sea of valence electrons. For these reasons, the actual results presented here are obtained by modeling the binary collision process as a collision between a neutral, inert gas atom and an ion core of the target atom. In the cases of copper and silver, the ion cores are fairly well defined, since both appear in column I.B. of the periodic table. However, in the cases of molybdenum and aluminum which appear in the VI.B. and III.A. columns of the periodic table, respectively, there are several possible ion core configurations that could be used in the HCM model. For this reason, various degrees of ionization of the molybdenum and aluminum target atoms were used in computing the SEE coefficient for these target atoms by way of the HCM model.

In the cases of copper and silver, results indicate that the best ion core configuration for both target materials is the singly ionized state. Note that all graph titles refer to the HCM model used, whereas the figure captions indicate the physical system actually investigated.

A. ANGULARLY DEPENDENT RESULTS

The results obtained from the bombardment of Cu single crystals by Ar ions for various angles of rotation about the <$\bar{1}$10> crystallographic axis are shown in Figure 17. It is interesting that the HCM model did not predict the correct behavior of the SEE coefficient for monocrystalline, angularly rotated targets, but did accurately reproduce the results obtained for polycrystalline targets [19]. This seems to indicate that the single collision model is not an accurate one for arbitrary rotations about the crystallographic axis, but needs to be modified to account for a more complicated interaction with the crystal lattice.

B. METAL TARGET RESULTS

An attempt was made in this thesis to verify those calculations performed by HCM in their original paper. Not too surprisingly, the results obtained here differ appreciably from those obtained by HCM using their original model. Each system is discussed in detail below.

1. Copper Bombarded by Ar, Ne, Kr and Xe Ions

In HCM's original paper, the Ar^+ - Cu system was treated in detail. Using their original model, they

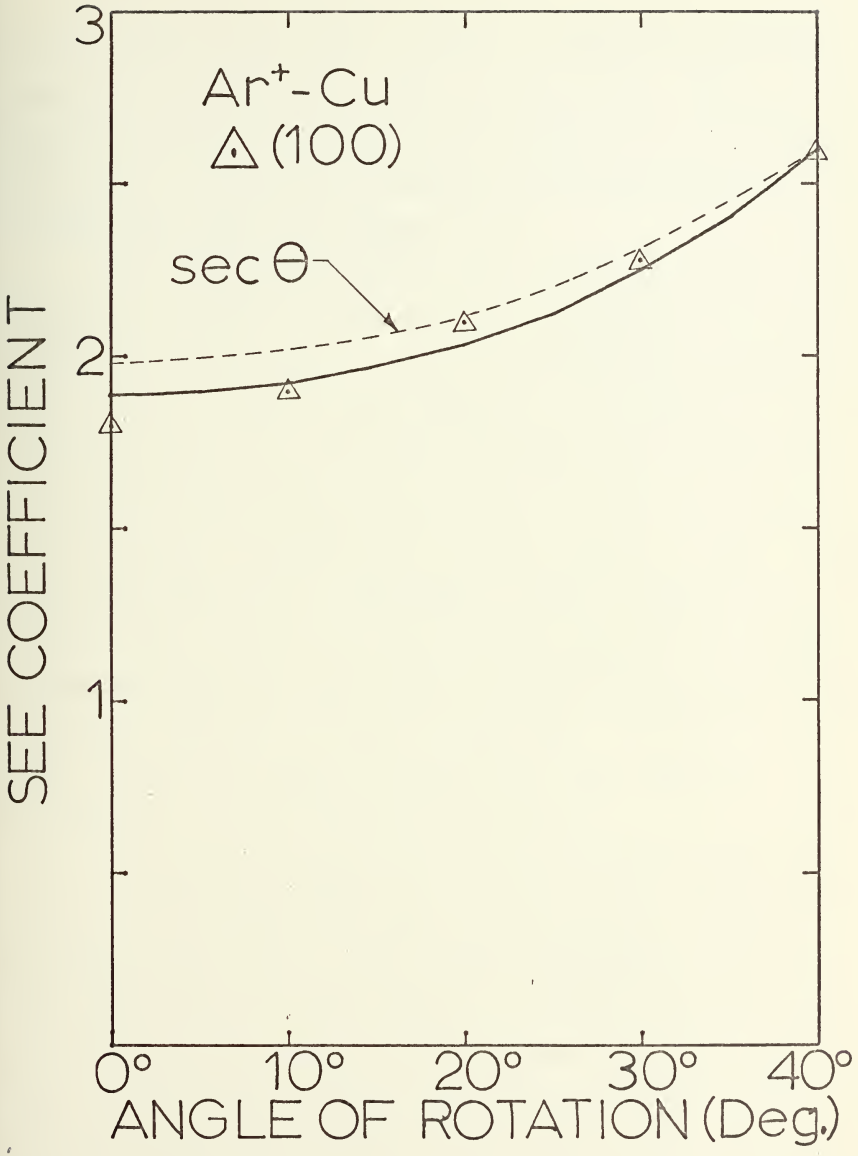

Figure 17. SEE coefficient vs. angle of rotation for (100) FCC Copper crystal. Direction of rotation was about <110>.

obtained the results shown in Figure 7, which show excellent agreement with experiment. After altering their model, using the modifications presented in Chapter IV, the results do not agree so well with experiment as did those obtained by HCM. (See Figures 18 through 21.)

In an attempt to explain this discrepancy, the difference between the experimentally observed SEE coefficient and that obtained here was plotted as a function of energy. Theoretically, if the results obtained in this present investigation are to be physically meaningful, this difference must be due to the potential ejection mechanism operating at higher energies. Experimentally, Medvel et al. [1] have ascertained that for Ar bombardment of polycrystalline Mo targets, the potential ejection mechanism is still operating at energies up to 2.5 Kev, and the PSE contribution is still tending to increase with increasing energy. If this is in fact the case, the results obtained here have physical significance. (See Figures 22 through 25.)

It is interesting to note that the PSE contribution from all three faces investigated exhibit similar behavior in that they all peak at approximately the same energy, and tend to decrease at higher energies. The exact location of the peak, however, varies with the primary ion type. Furthermore, in all four primary ion cases, the PSE contribution curves for the (100) and (110) faces cross at approximately seven to nine Kev, indicating that the PSE mechanism may be somewhat independent of ion type, while showing some

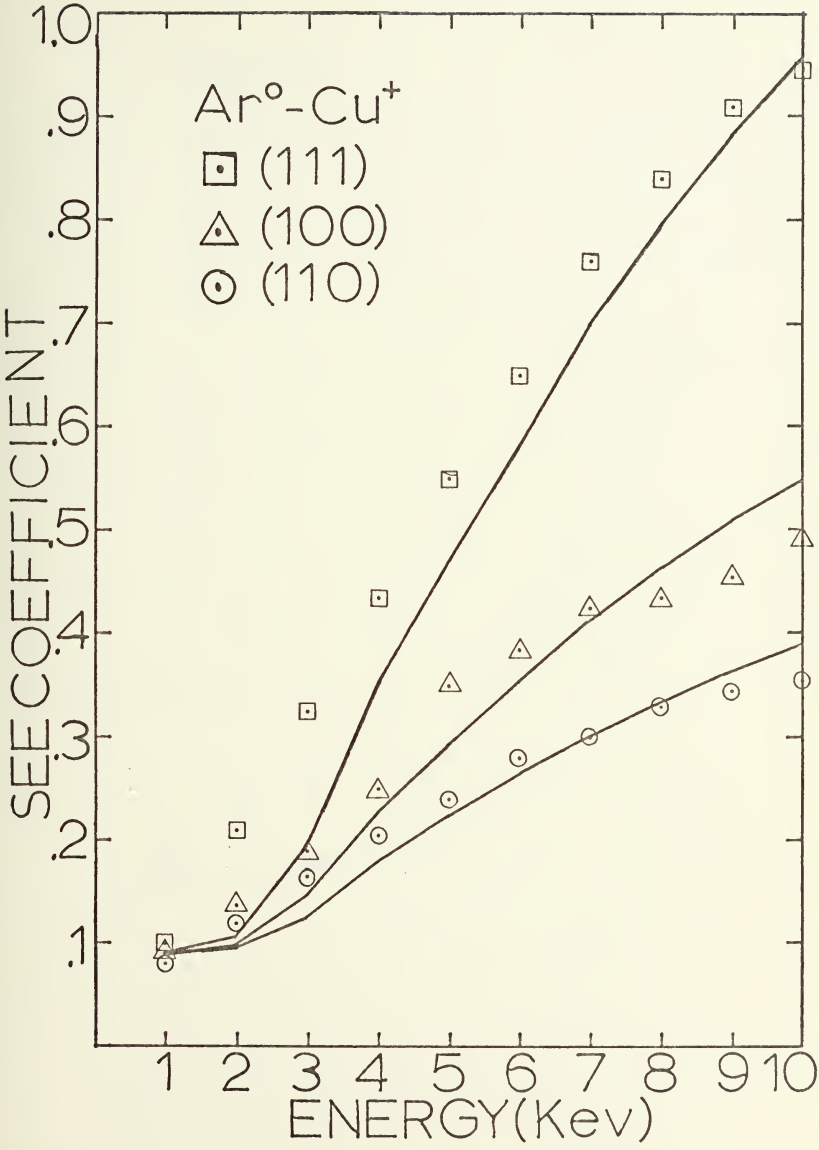

Figure 18. Cu bombarded by Ar^+ ions normally incident on the (100), (110) and (111) planes.

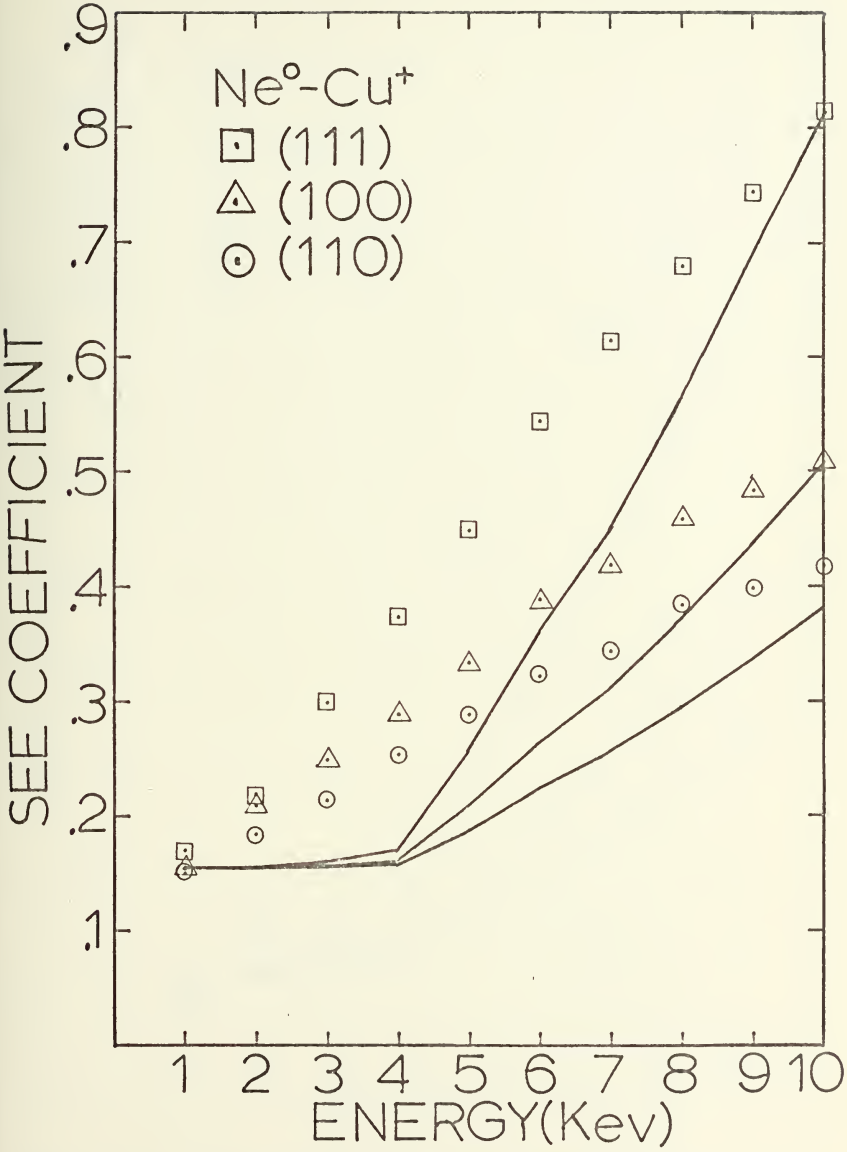

Figure 19. Cu bombarded by Ne^{+} ions normally incident on the (100), (110) and (111) faces.

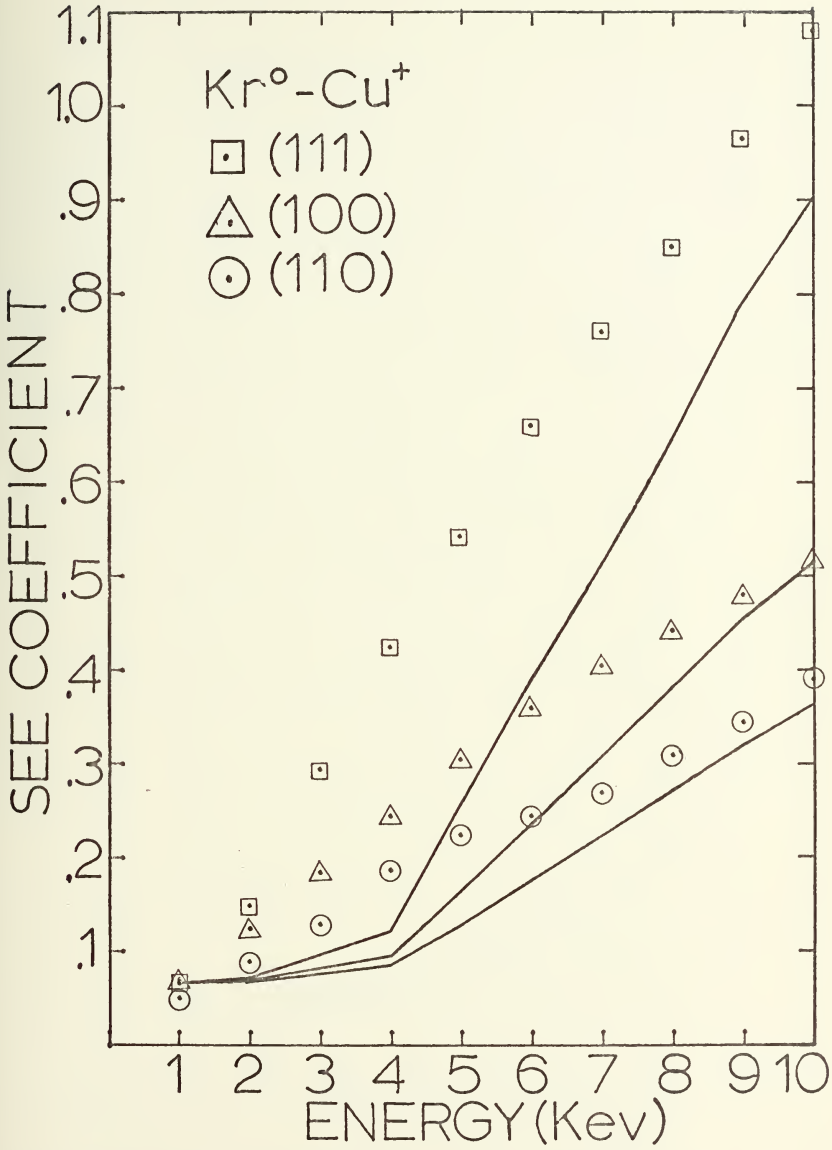

Figure 20. Cu bombarded by Kr^+ ions normally incident on the (100), (110) and (111) faces.

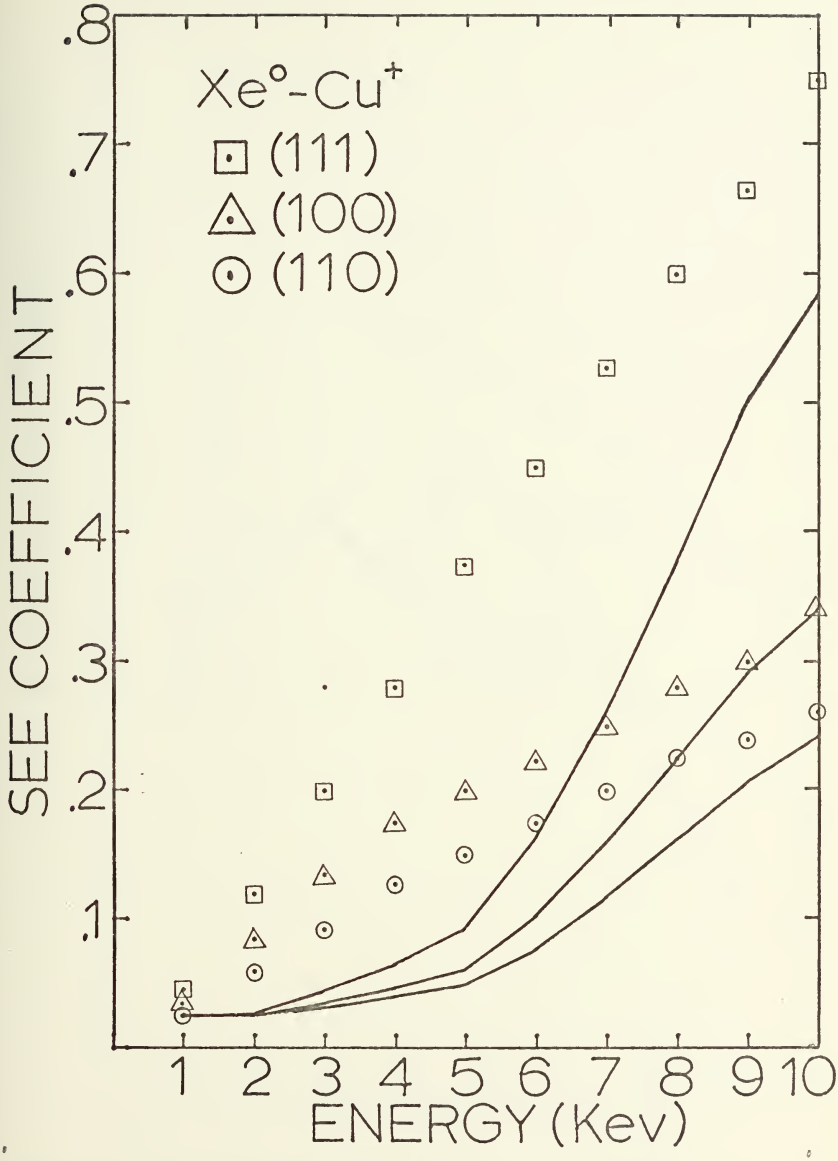

Figure 21. Cu bombarded by Xe^{+} ions normally incident on the (100), (110) and (111) faces.

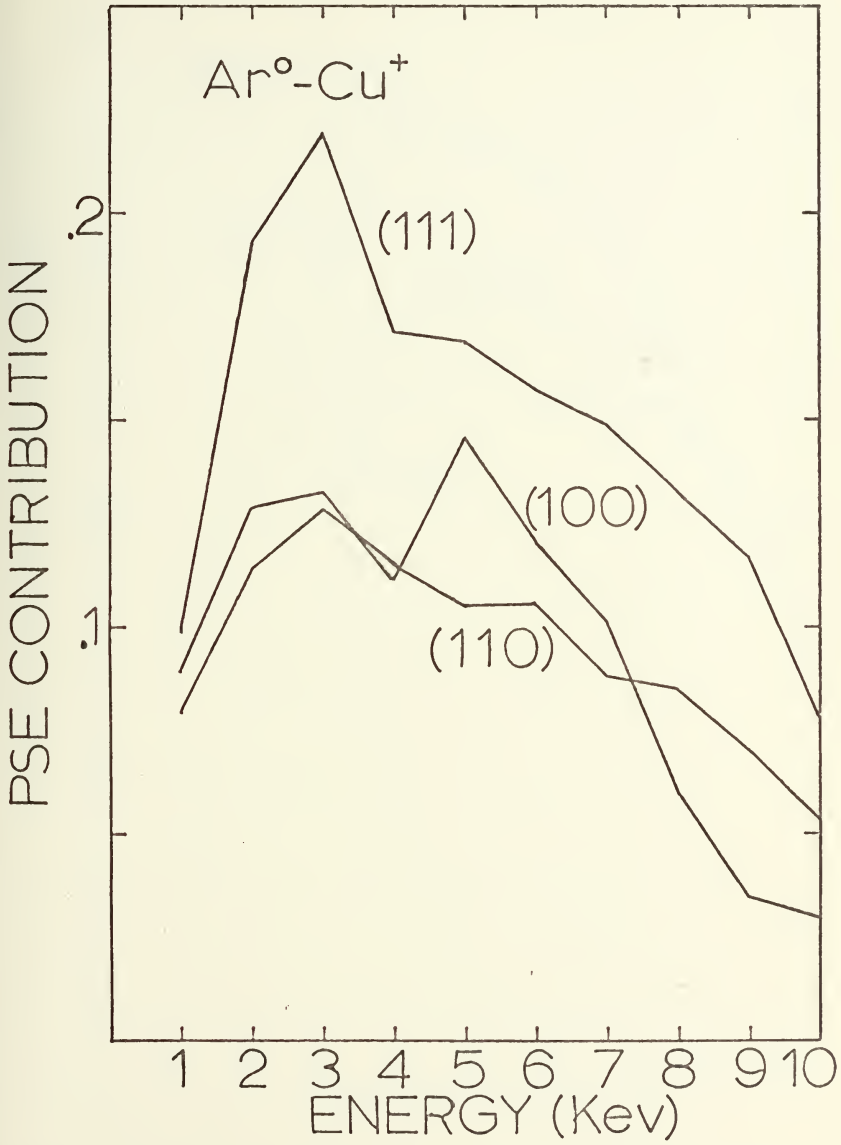

Figure 22. PSE contribution to secondary electron emission for the Ar^{+} - Cu system.

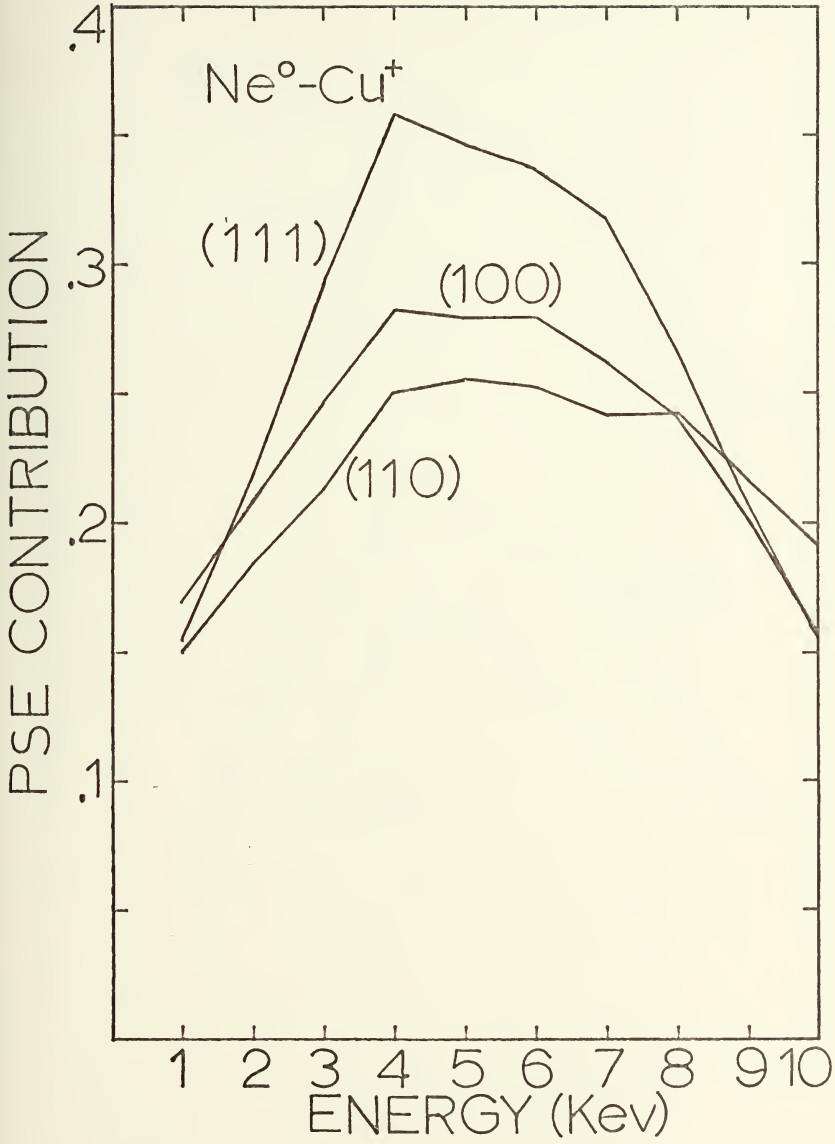

Figure 23. PSE contribution to secondary electron emission for the Ne^{+} - Cu system.

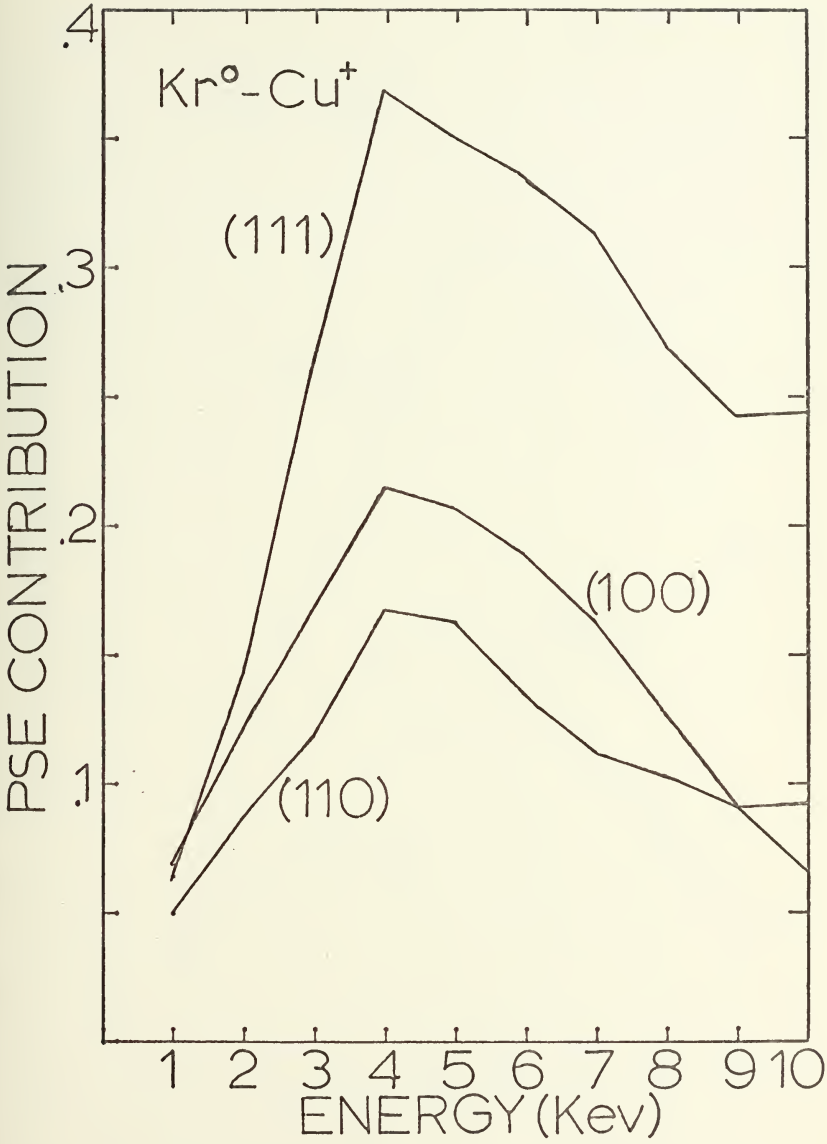

Figure 24. PSE contribution to secondary electron emission for the Kr^{+} - Cu system.

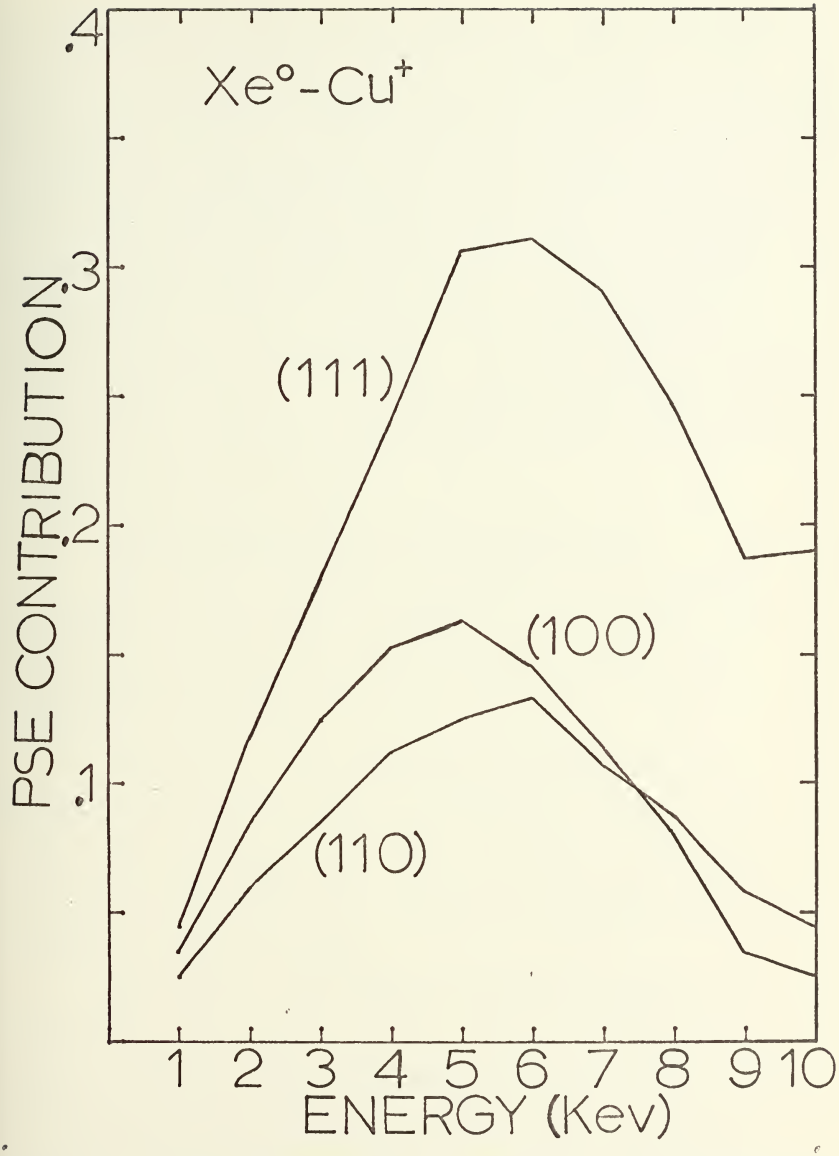

Figure 25. PSE contribution to secondary electron emission for the Xe^{+} - Cu system.

dependence on the plane being bombarded. Such a crossing behavior in the PSE contribution as a function of energy would not be expected simply by analyzing the SEE coefficient curves, since these curves do not cross at any energy. If this is the case, then it would follow that the theoretical results obtained for each crystal face should be independently fitted to the experimental data, without regard to the other planes being bombarded. In most cases this would yield results that are in closer agreement with experiment and yet do not eliminate the PSE contribution to secondary electron emission entirely.

2. Silver Bombarded by Ar, Ne, and Kr Ions

The silver systems also indicate the possibility of the PSE mechanism being dependent on the crystal face being bombarded as well as the primary ion type. (See Figures 26 through 31.)

In the Ar^+ - Ag system the PSE contribution to secondary electron emission is initially largest for the (100) face, followed by the (111) and (110) faces, respectively. In all three cases the PSE contribution decreases slightly at higher energies.

In the Kr^+ - Ag system a different ordering of facial PSE contributions appear. Initially, the (111) face contributes the most to potential emission, followed by the (100) and (110) faces, in that order. At higher energies, the ordering changes, with (100) contributing the largest amount to PSE, followed by (111) and (110),

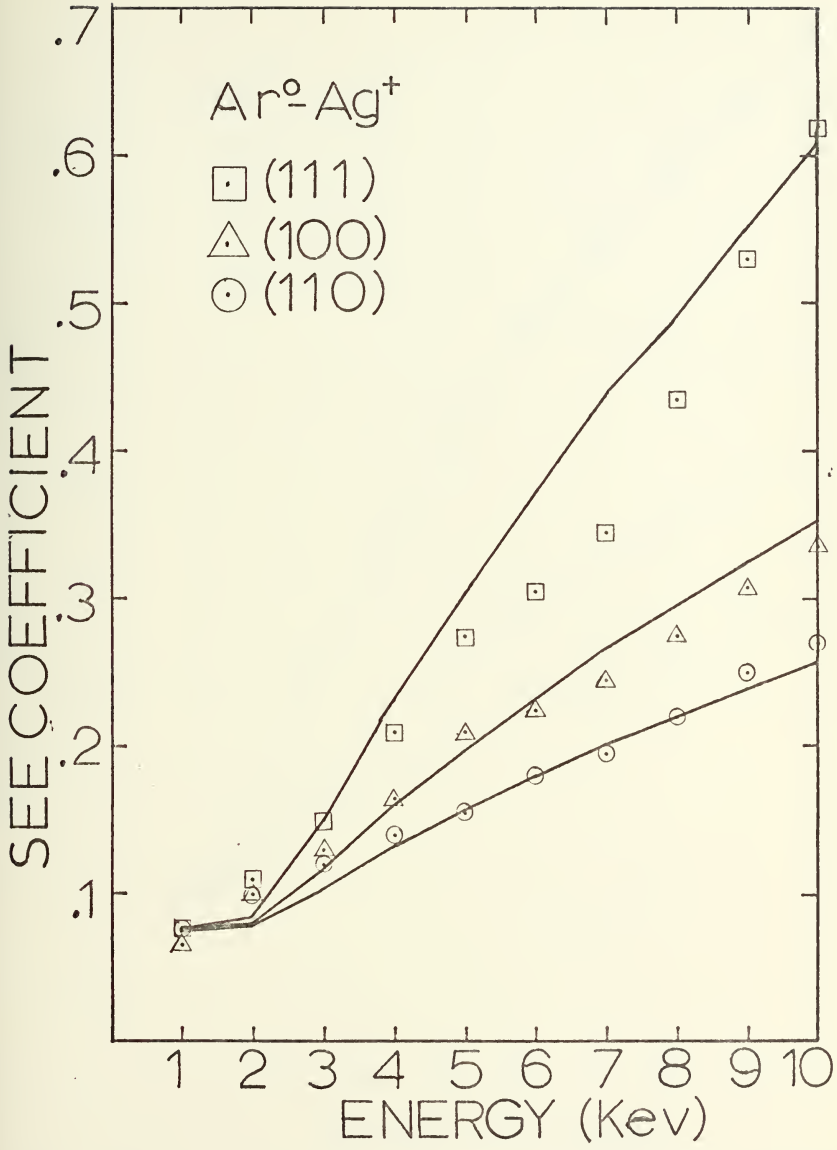

Figure 26. Ag bombarded by Ar^+ ions normally incident on the (100), (110) and (111) faces.

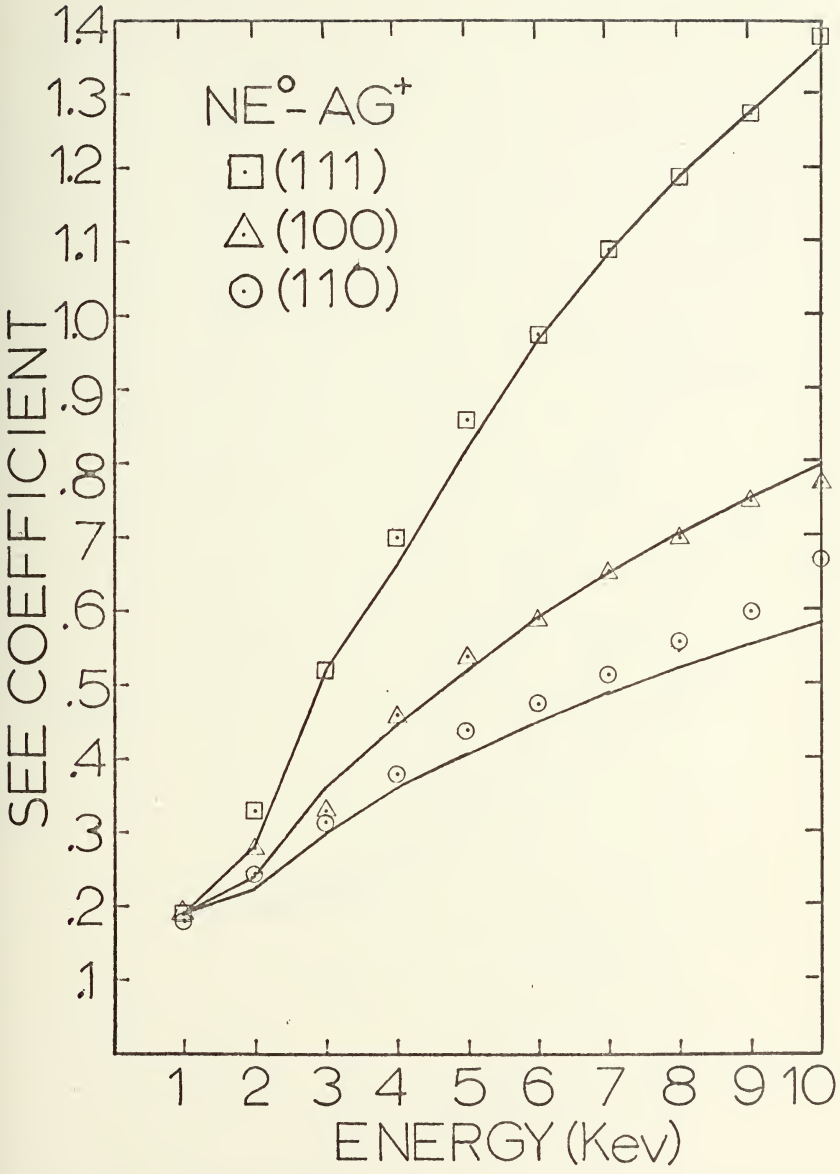

Figure 27. Ag bombarded by Ne^{+} ions normally incident on the (100), (110) and (111) faces.

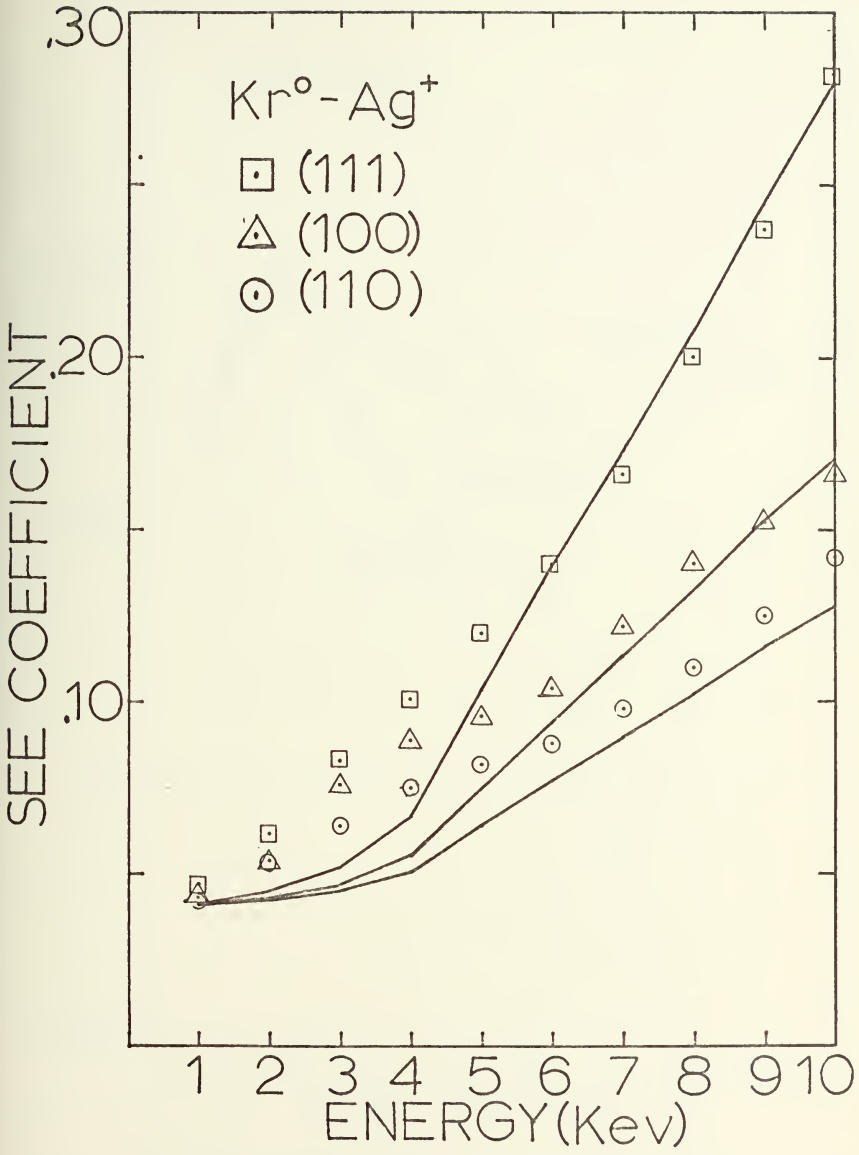

Figure 28. Ag bombarded by Kr^+ ions normally incident on the (100), (110) and (111) faces.

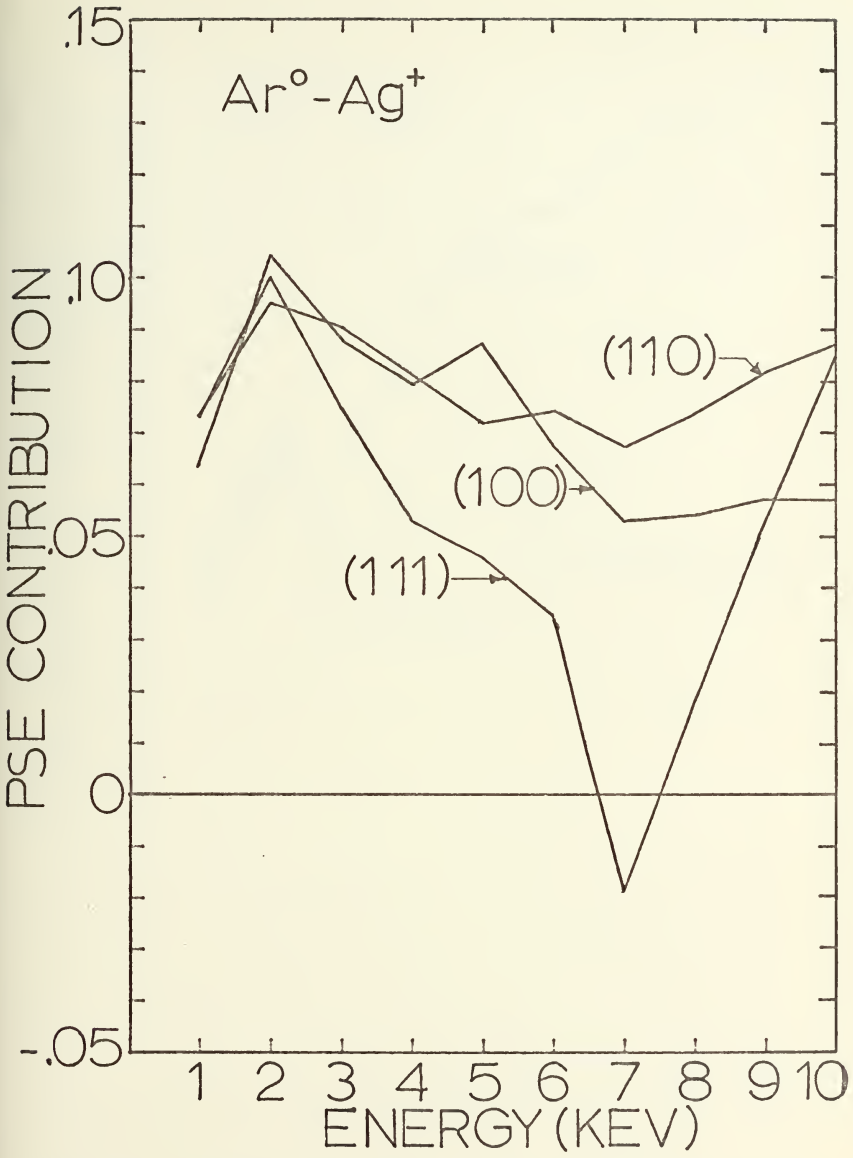

Figure 29. PSE contribution to secondary electron emission for the Ar^{+} - Ag system.

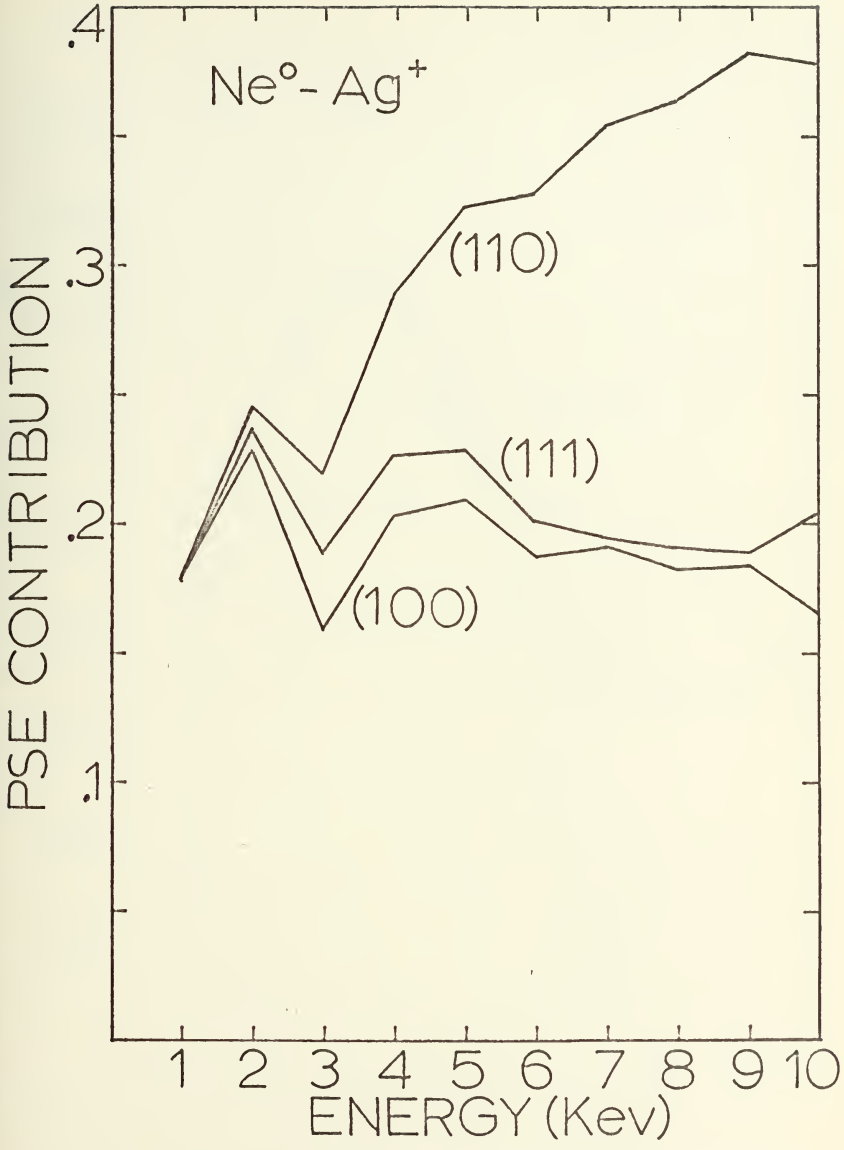

Figure 30. PSE contribution to secondary electron emission for the Ne^{+} - Ag system.

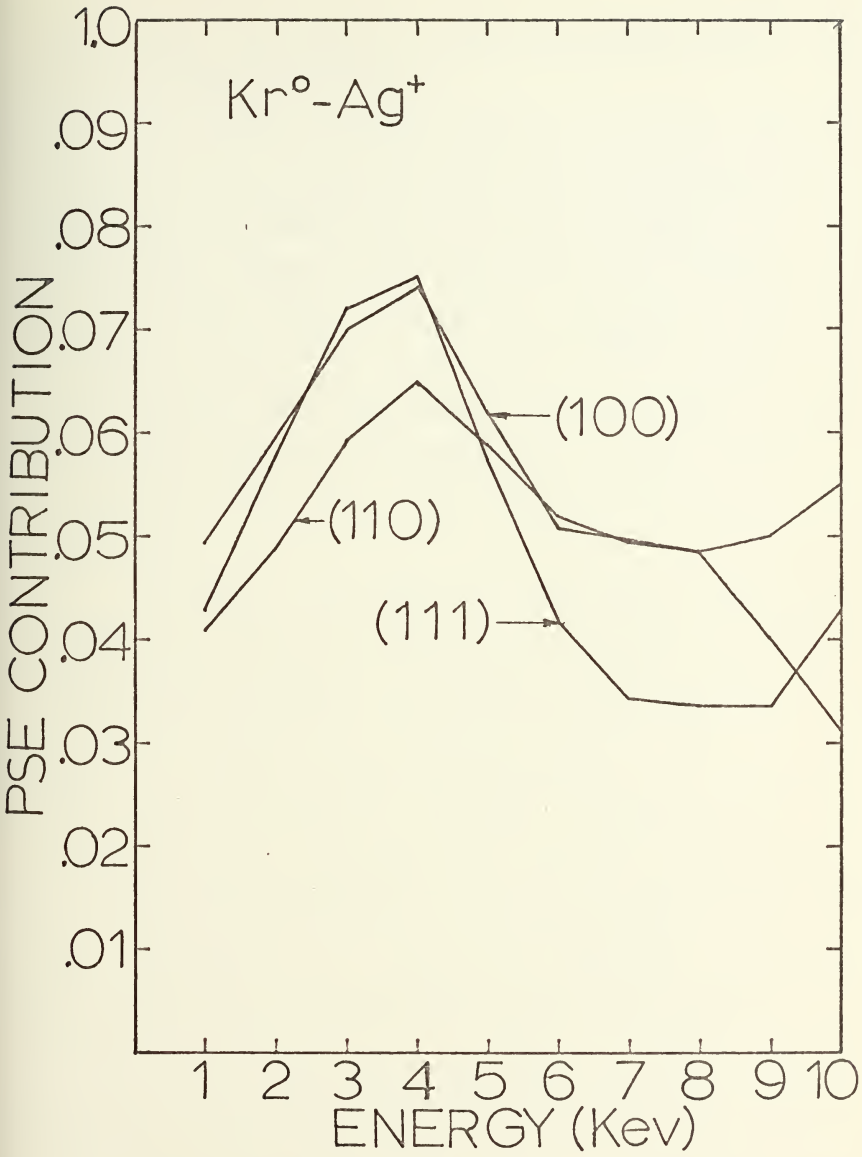

Figure 31. PSE contribution to secondary electron emission for the Kr^{+} - Ag system.

respectively. Once again, the PSE contribution tends to decrease at higher energies.

In the Ne^+ - Ag system an entirely different picture arises. For all energies, the (110) face contributes the most to PSE, followed by the (111) and (100) faces, respectively. However, even at ten Kev, the potential emission for the (110) face is still rising whereas, over the entire energy range, the PSE contribution from the (111) and (100) face remains fairly constant. These results would seem to indicate, once again, that not only is potential emission dependent on primary ion type, but also on crystal face.

In the Ar^+ - Ag system, the PSE contribution from the (111) face goes to a negative value at seven Kev. The reason for this behavior can be found by analyzing the Ar^+ - Ag SEE coefficient versus energy curves shown in Figure 26. The SEE coefficient experimental data for the (111) face dips downward at seven Kev. This behavior is not demonstrated on the other faces and would tend to indicate that some experimental variation may be present in these experimental data. On the other hand, the interaction being modeled may be sufficiently complicated that the potential contribution cannot be separated simply by scaling the results. No other system investigated displays similar results.

3. Molybdenum Bombarded by Ar, Ne, Kr and Xe Ions

In Figures 32 through 43, Mo^+ initially seems to be the ion core model that best represents secondary electron emission from various target faces. This conclusion holds true for the Ne^+ - Mo and Kr^+ - Mo systems. However, for the Xe^+ - Mo system, the best ion core model is not Mo^+ but Mo^{++}. This would seem to indicate that the primary ion type plays an important role in secondary electron emission.

4. Aluminum Bombarded by Ar, Kr, and Xe Ions

In the case of aluminum bombarded by Ar^+ (Figures 44 through 52) the Al^+ and Al^{++} ion core models for the target atoms yielded results that were almost identical. This system is contrasted with the Kr^+ - Al system which shows a distinct preference for Al^{++} as the ion core model, with the Al^+ and Al^{+++} yielding similar and uniformly poor results. Similarly, the Xe^+ - Al system shows the same preference for the Al^{++} ion core model and demonstrates a poorer fit when the Al^+ and Al^{+++} models are used. When all cases are considered, it would seem that secondary electron emission is sensitive to the primary ion type, as has been demonstrated by previous results.

C. ALKALI-HALIDE RESULTS

Experimental results for the bombardment of alkali-halide single crystals by inert gas ions have been obtained from experiments by Baboux and Pedrix [21, 22]. Two cases are considered in this present investigation. These include

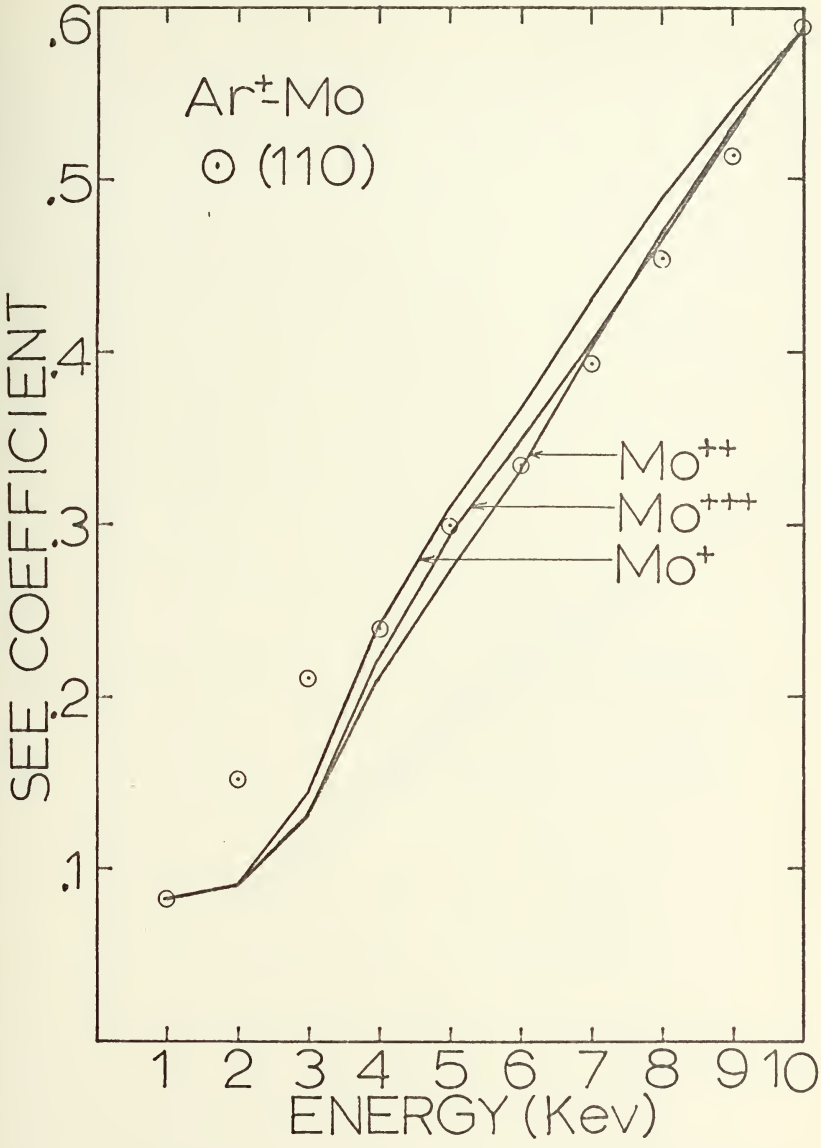

Figure 32. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Ar^{+} - Mo system.

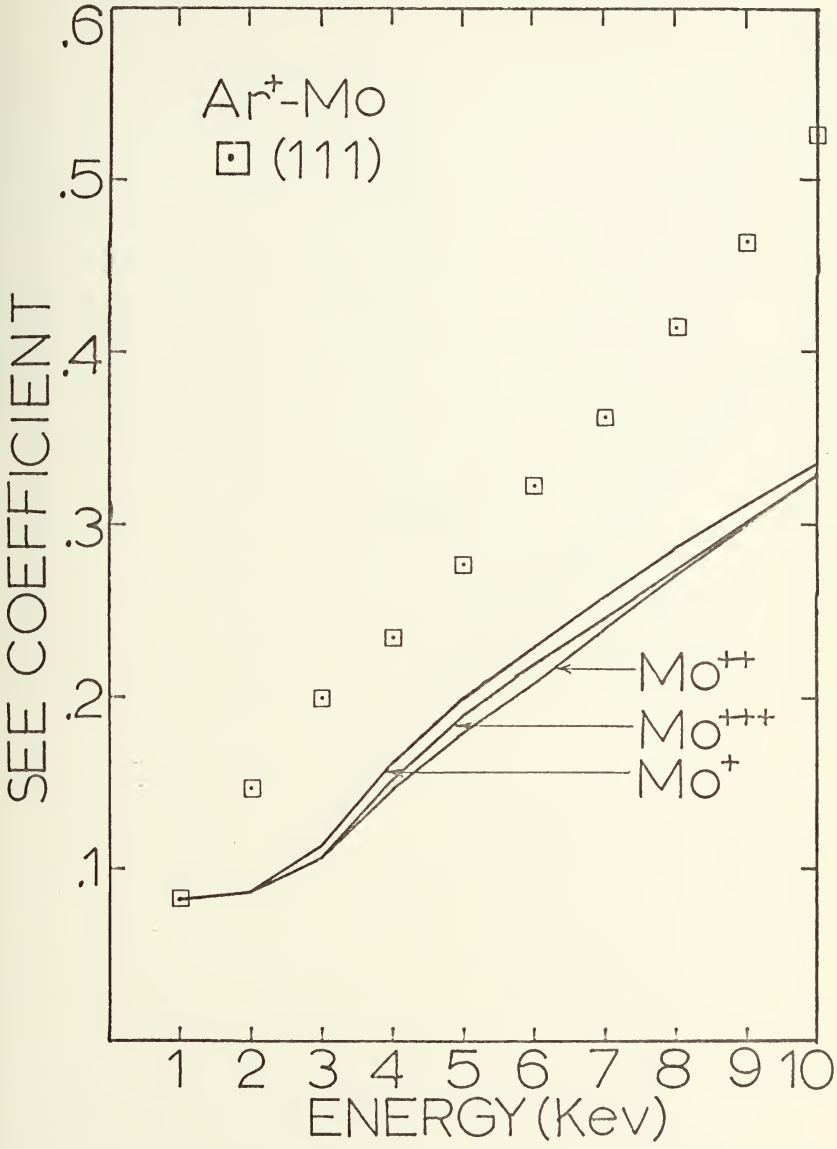

Figure 33. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Ar^+ - Mo system.

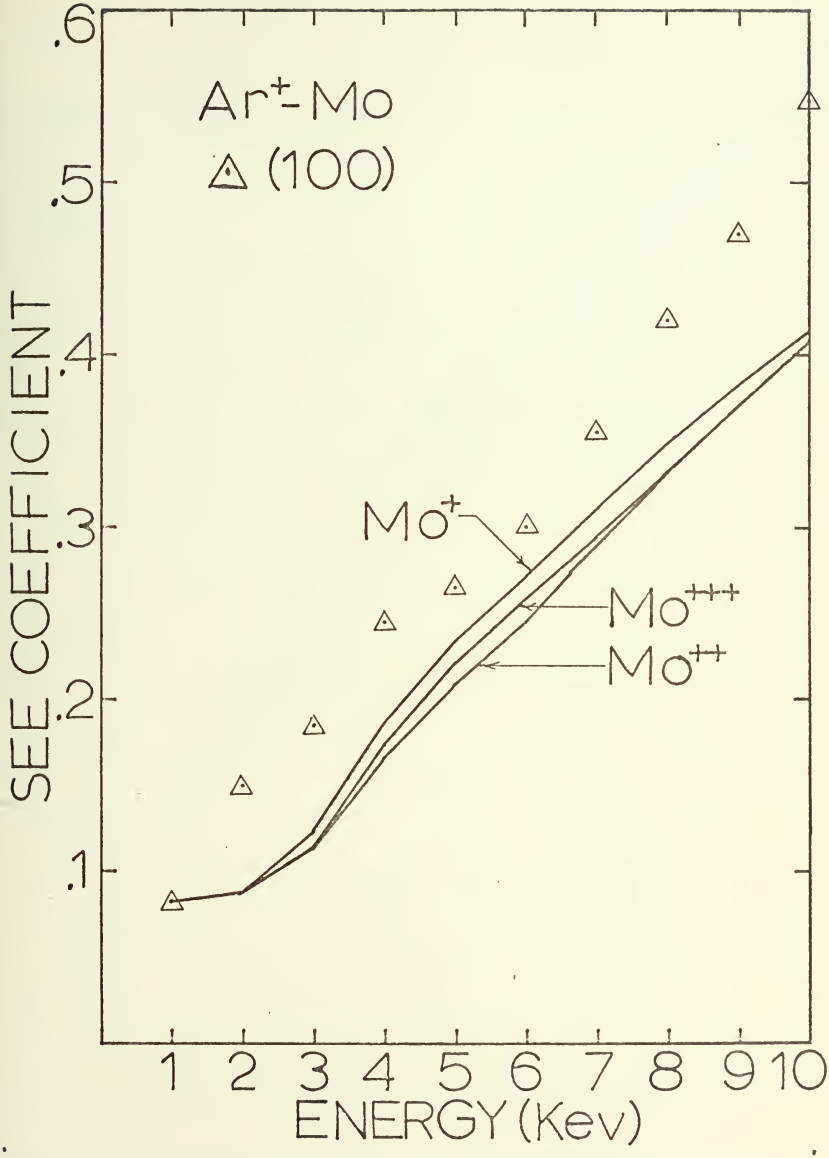

Figure 34. Effect of varying target atom ionization in the HCM model on secondary electron emission in the Ar^+ - Mo system.

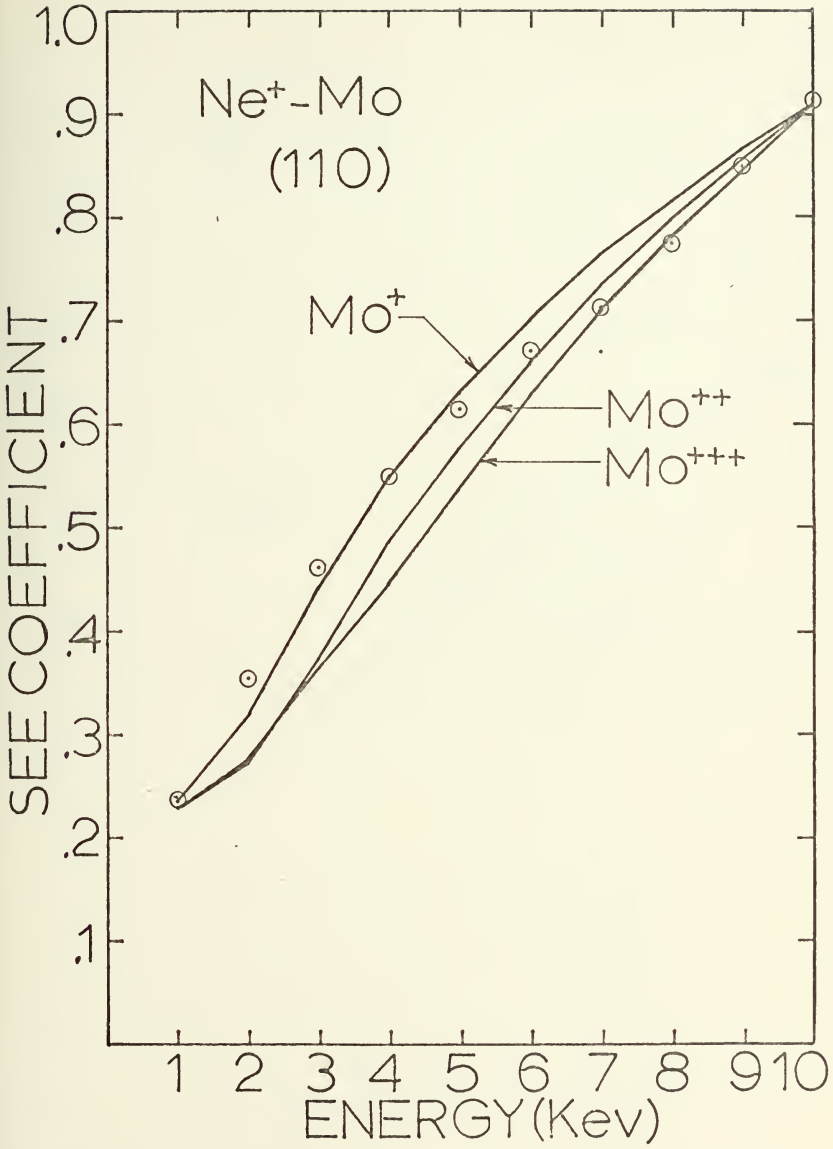

Figure 35. Effect on varying target atom ionization in the HCM model on secondary electron emission from the Ne^{+} - Mo system.

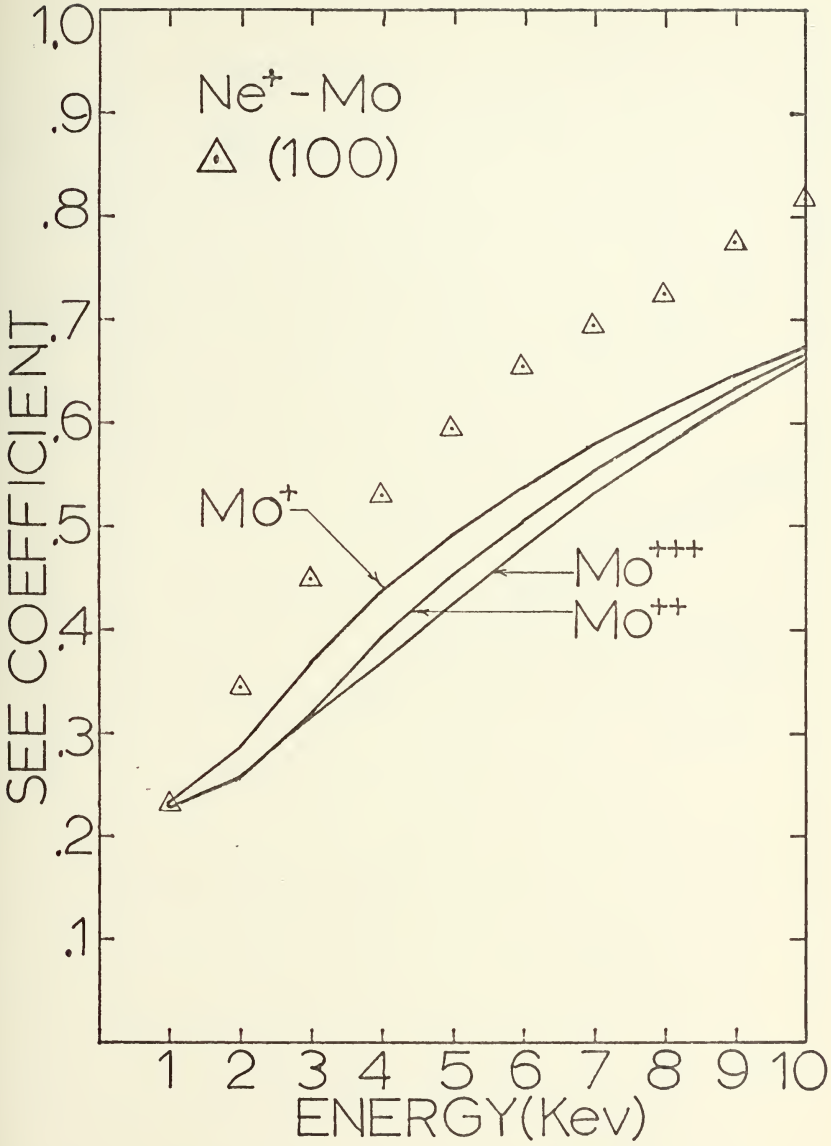

Figure 36. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Ne^{+} - Mo system.

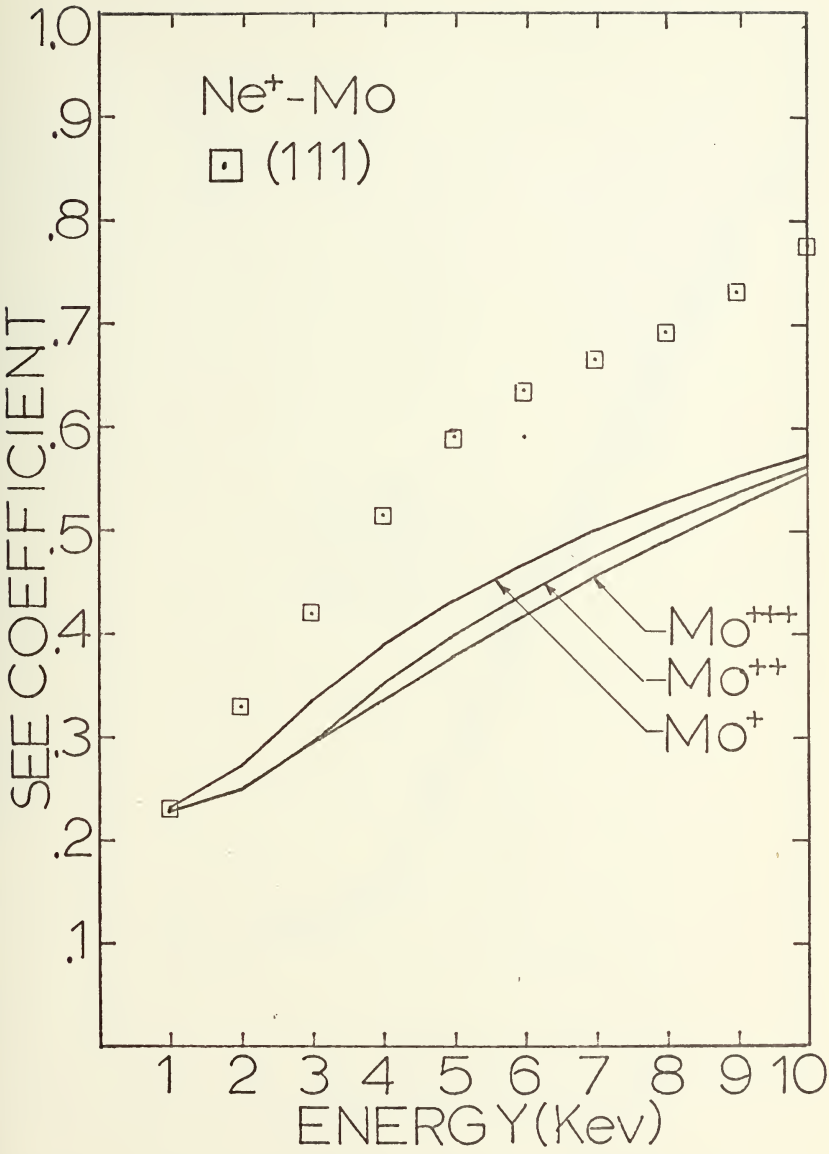

Figure 37. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Ne^{+} - Mo system.

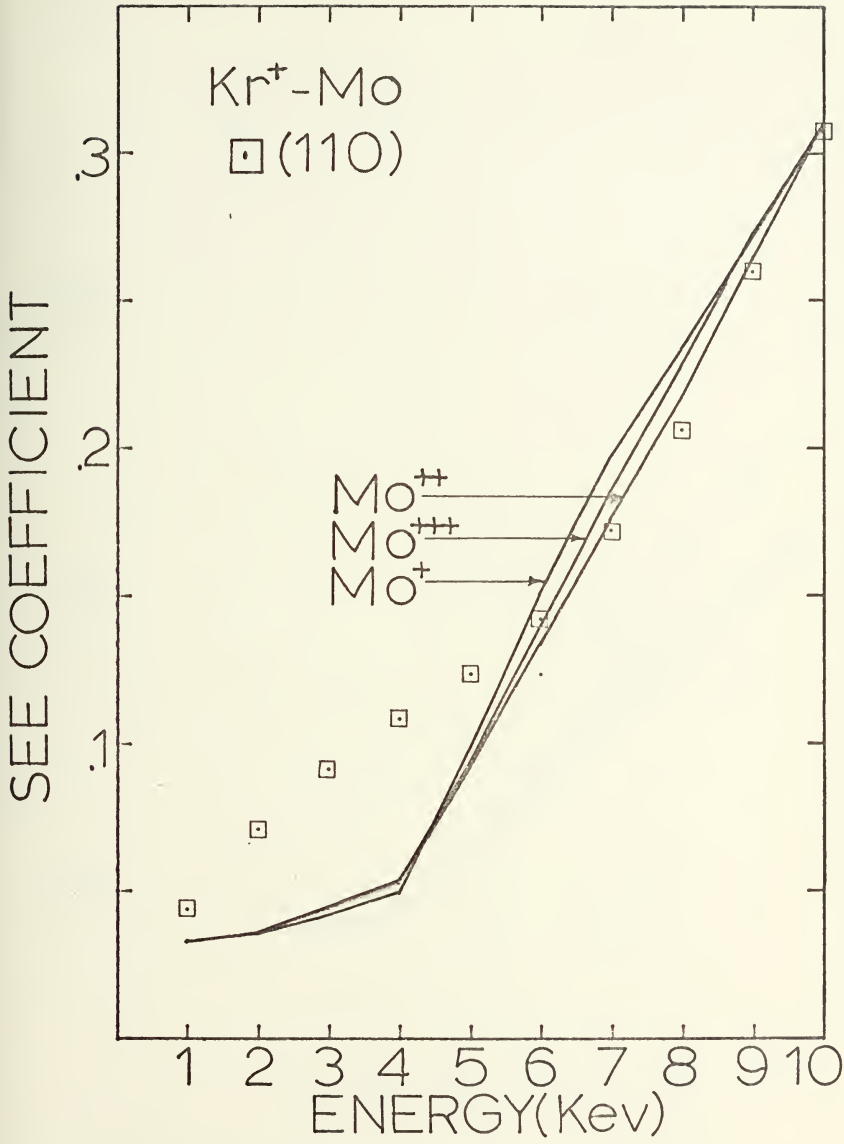

Figure 38. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Kr^{+} - Mo system.

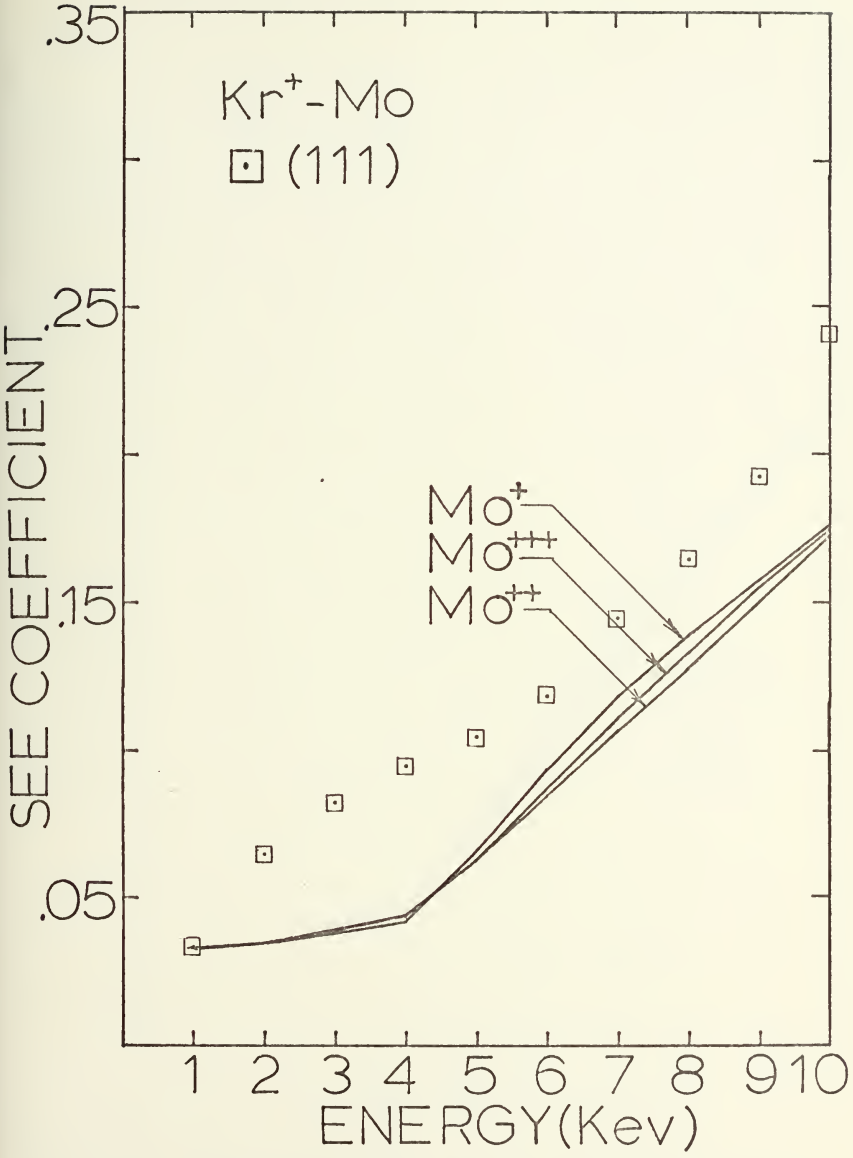

Figure 39. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Kr^{+} - Mo system.

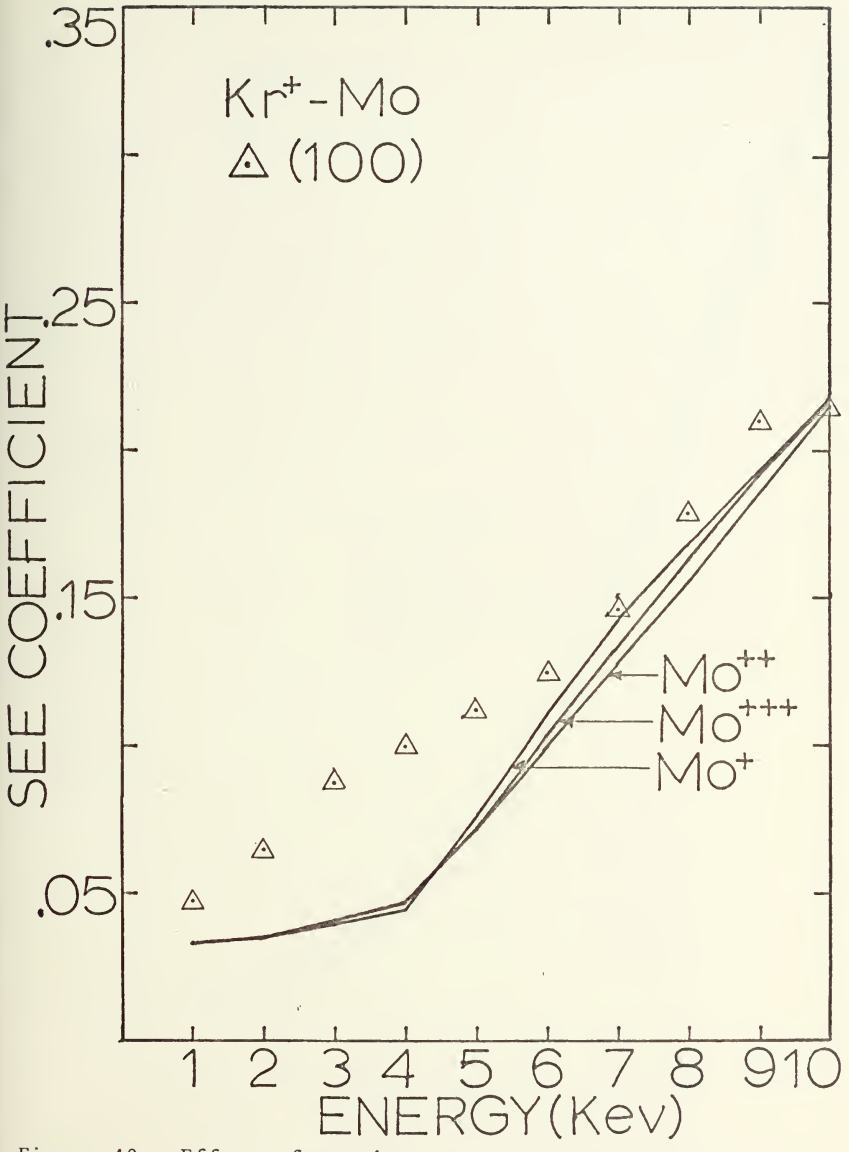

Figure 40. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Kr^{+} - Mo system.

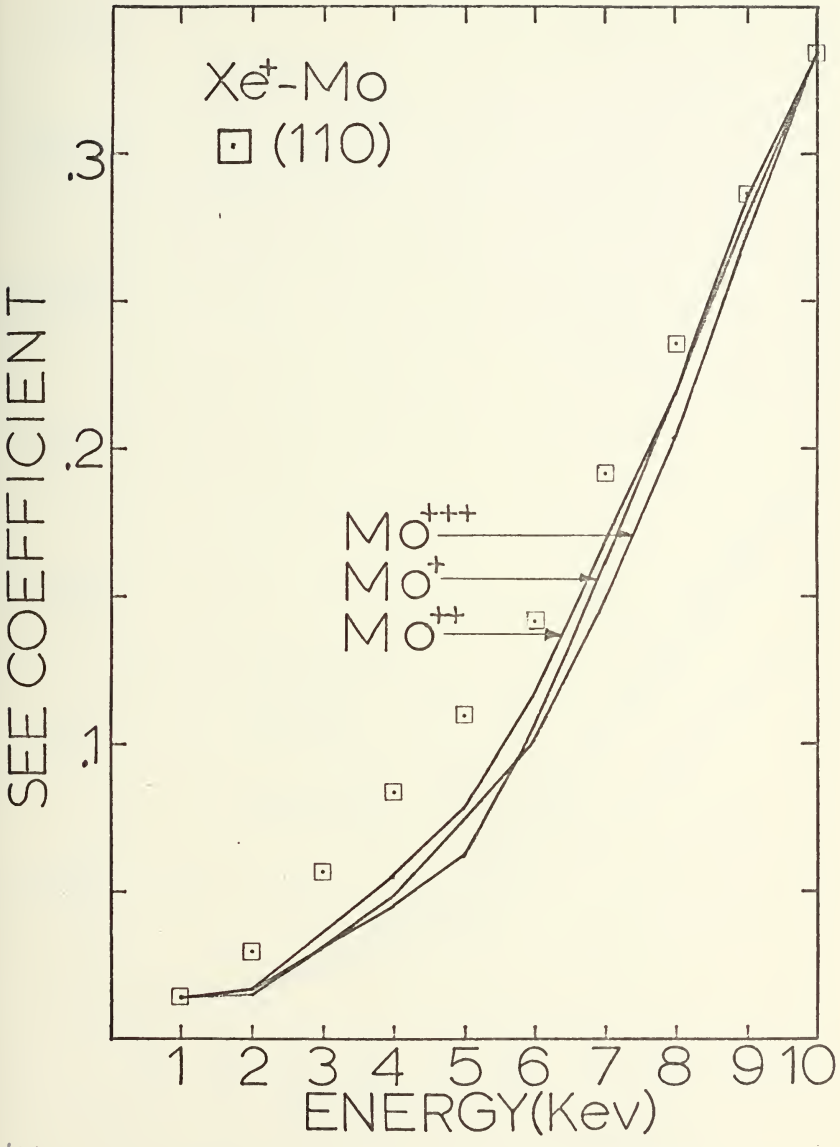

Figure 41. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Xe^{+} - Mo system.

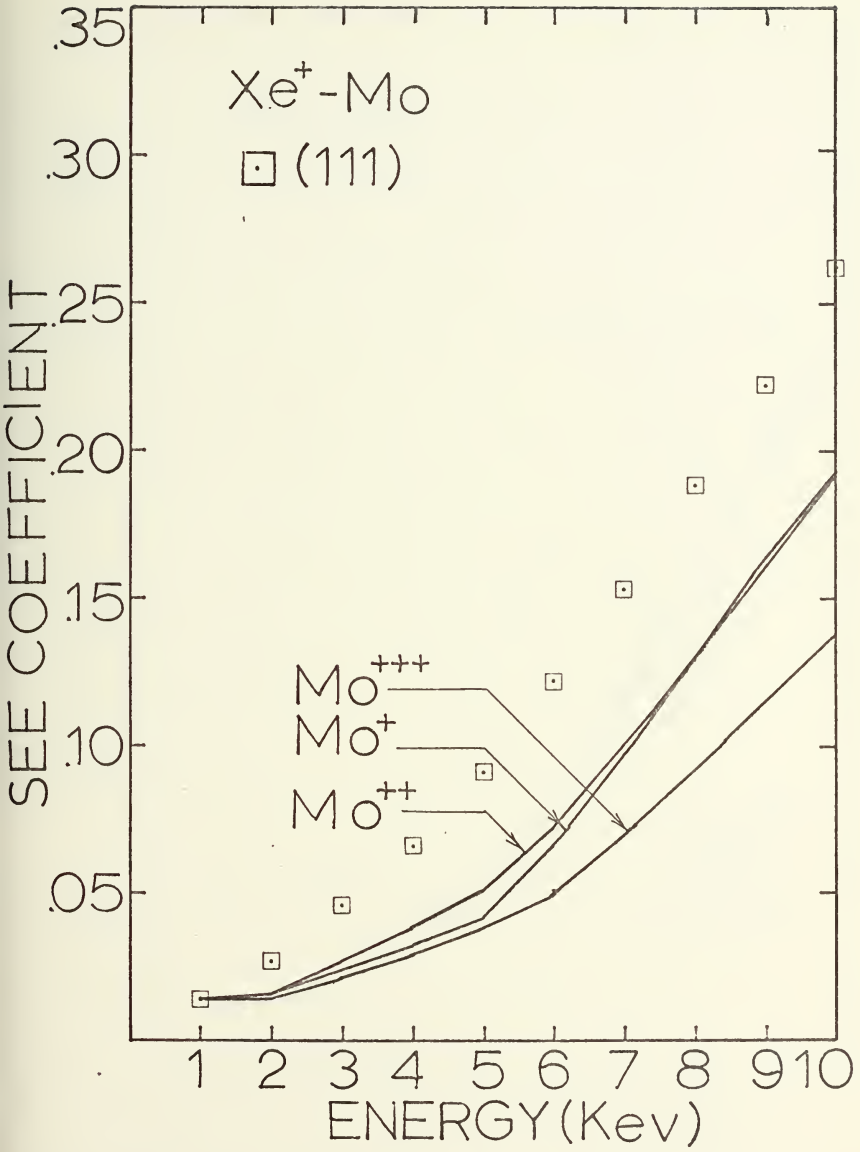

Figure 42. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Xe^{+} - Mo system.

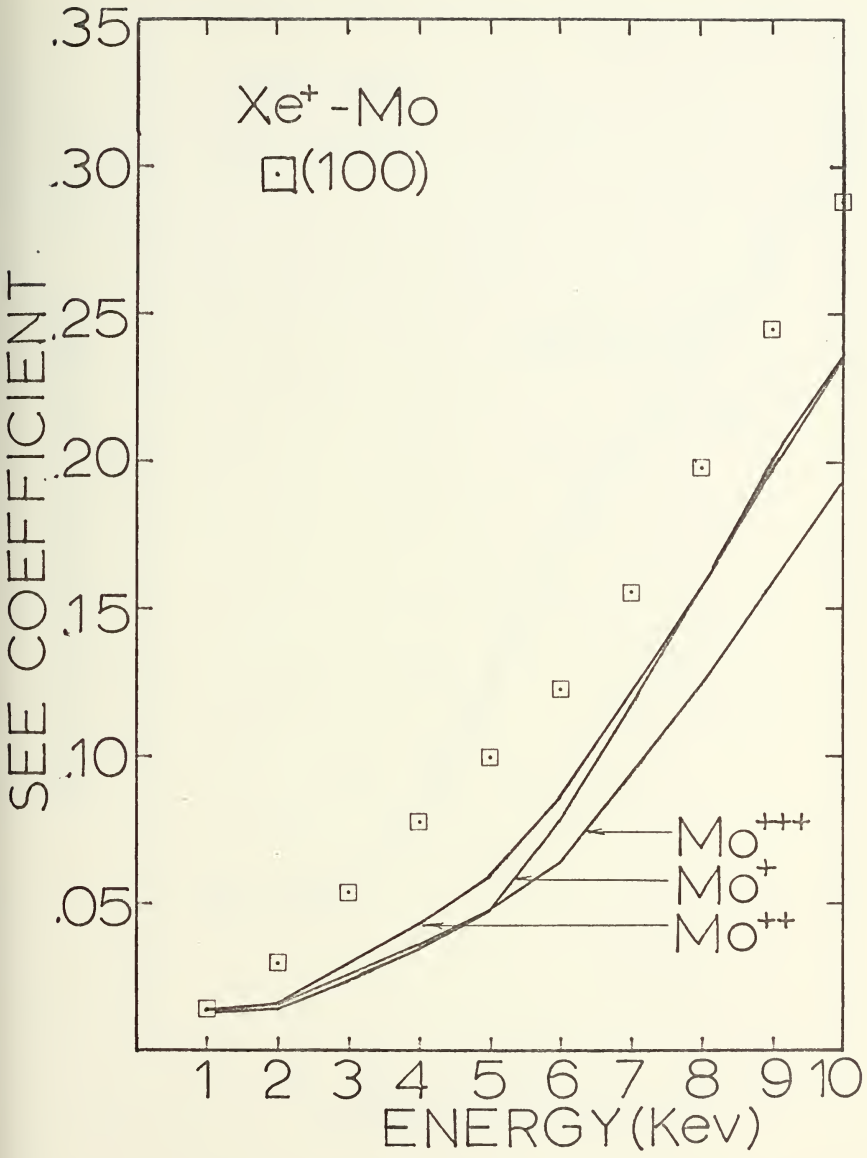

Figure 43. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Xe^{+} - Mo system.

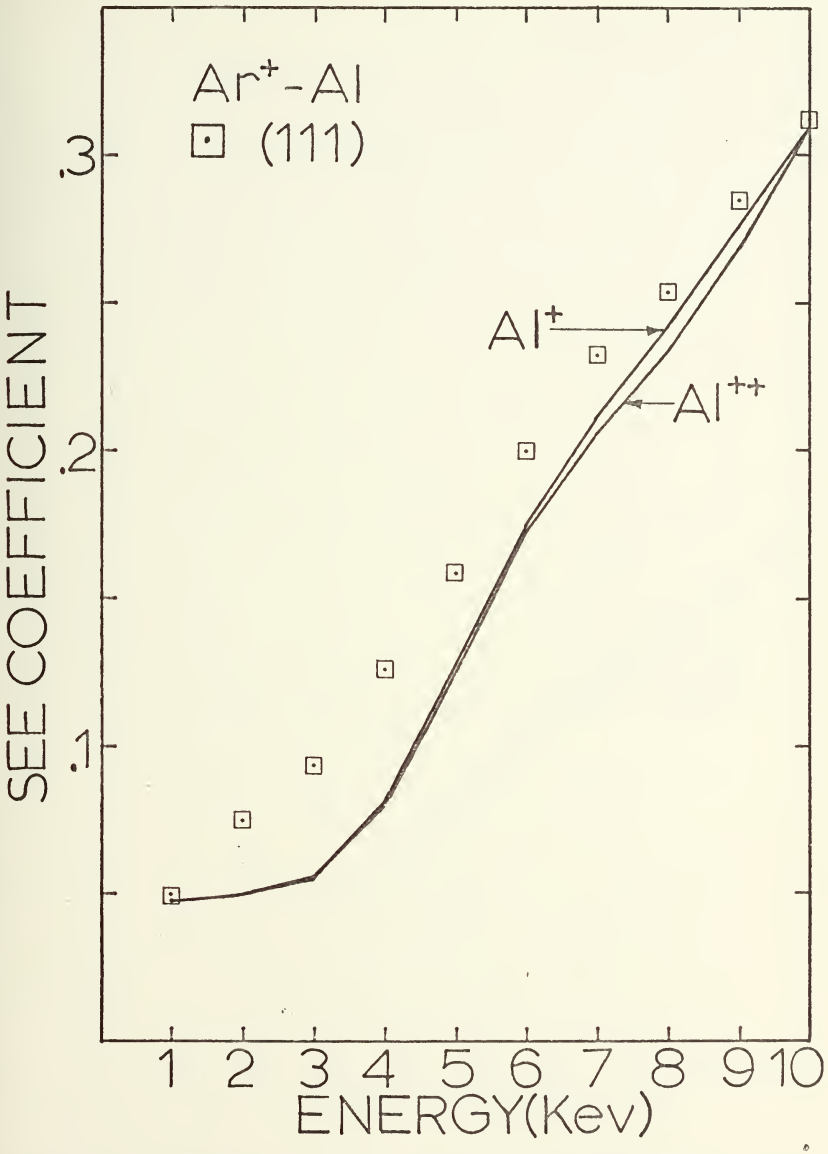

Figure 44. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Ar^+ - Al system.

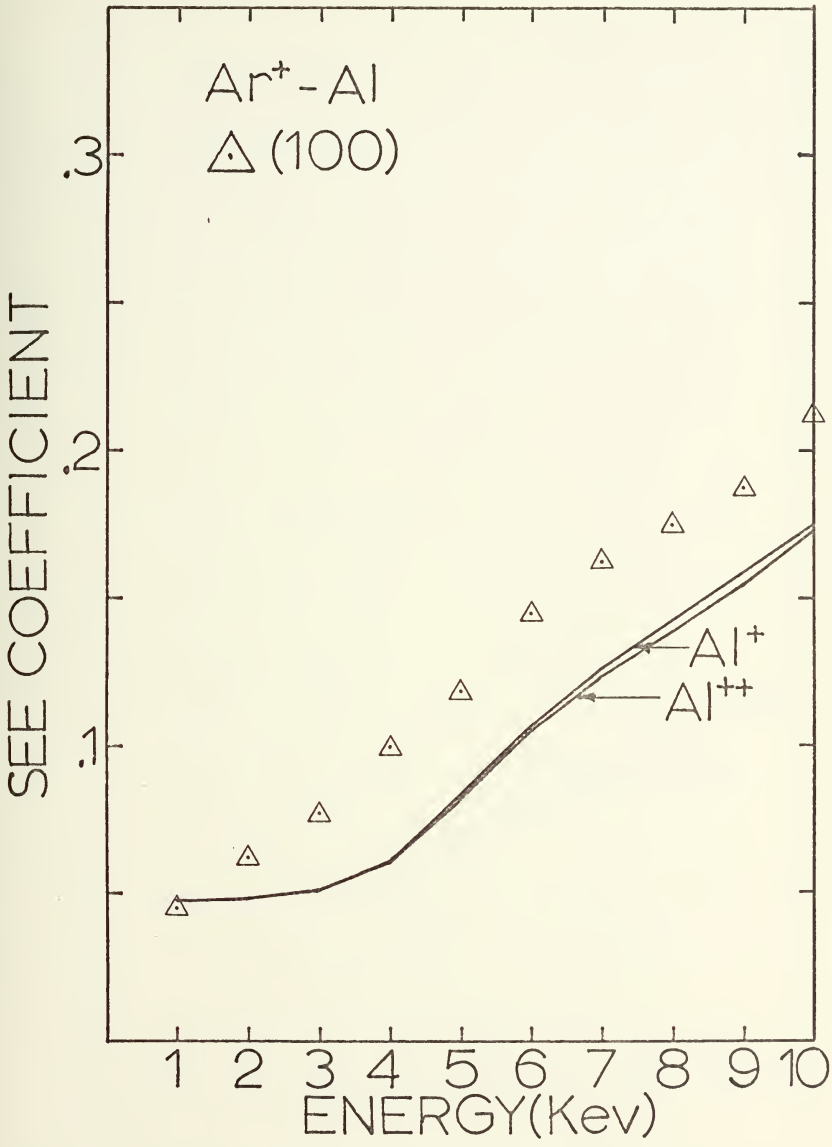

Figure 45. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Ar^{+} - Al system.

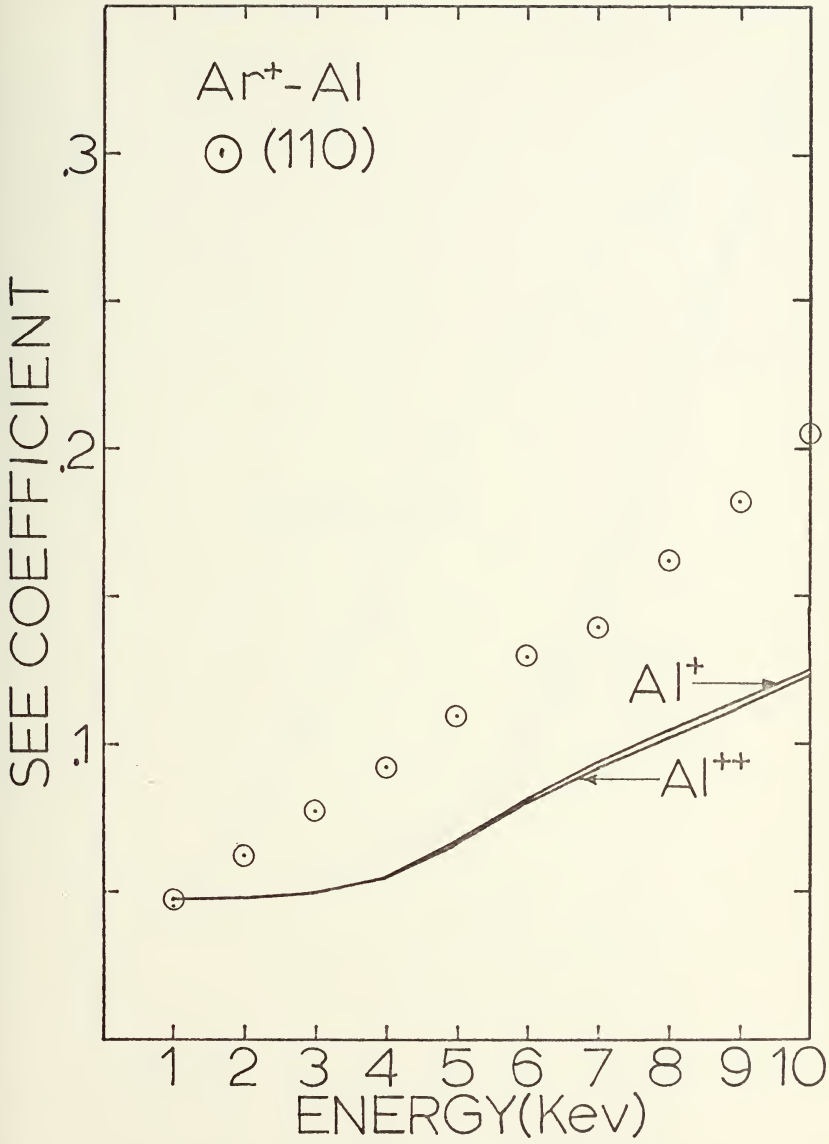

Figure 46. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Ar^{+} - Al system.

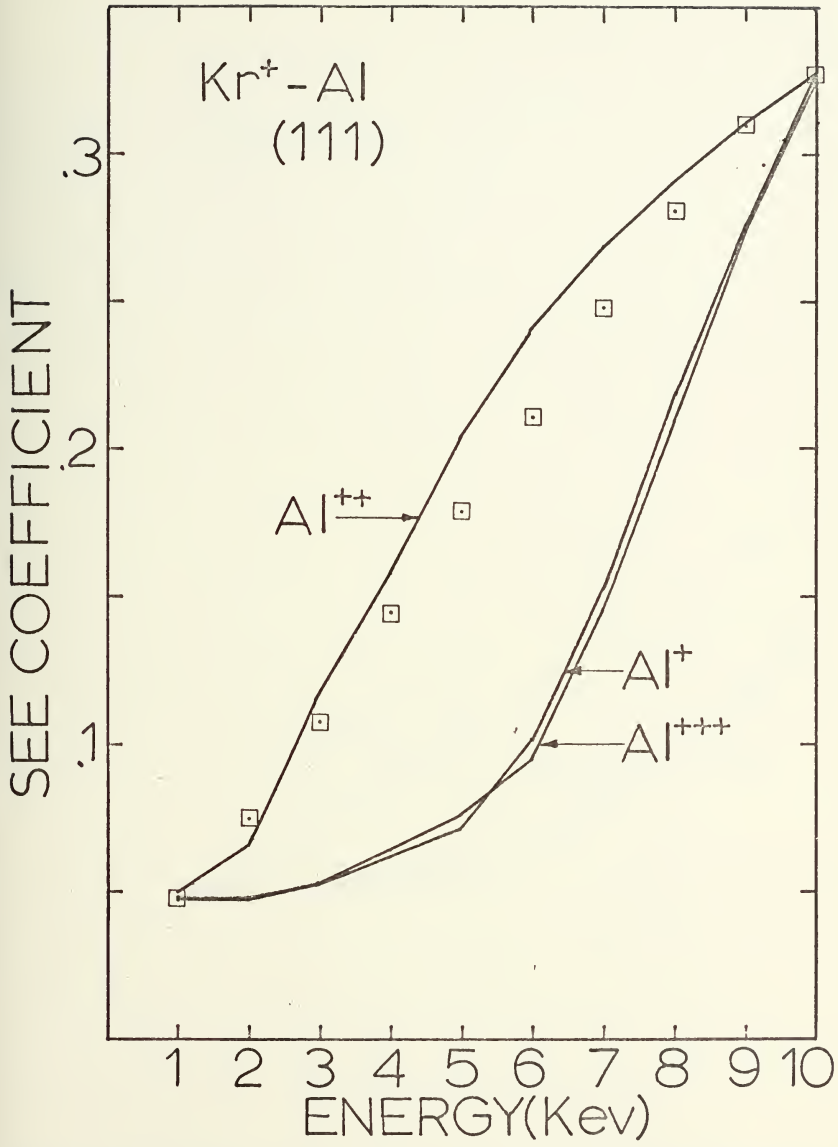

Figure 47. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Kr^{+} - Al system.

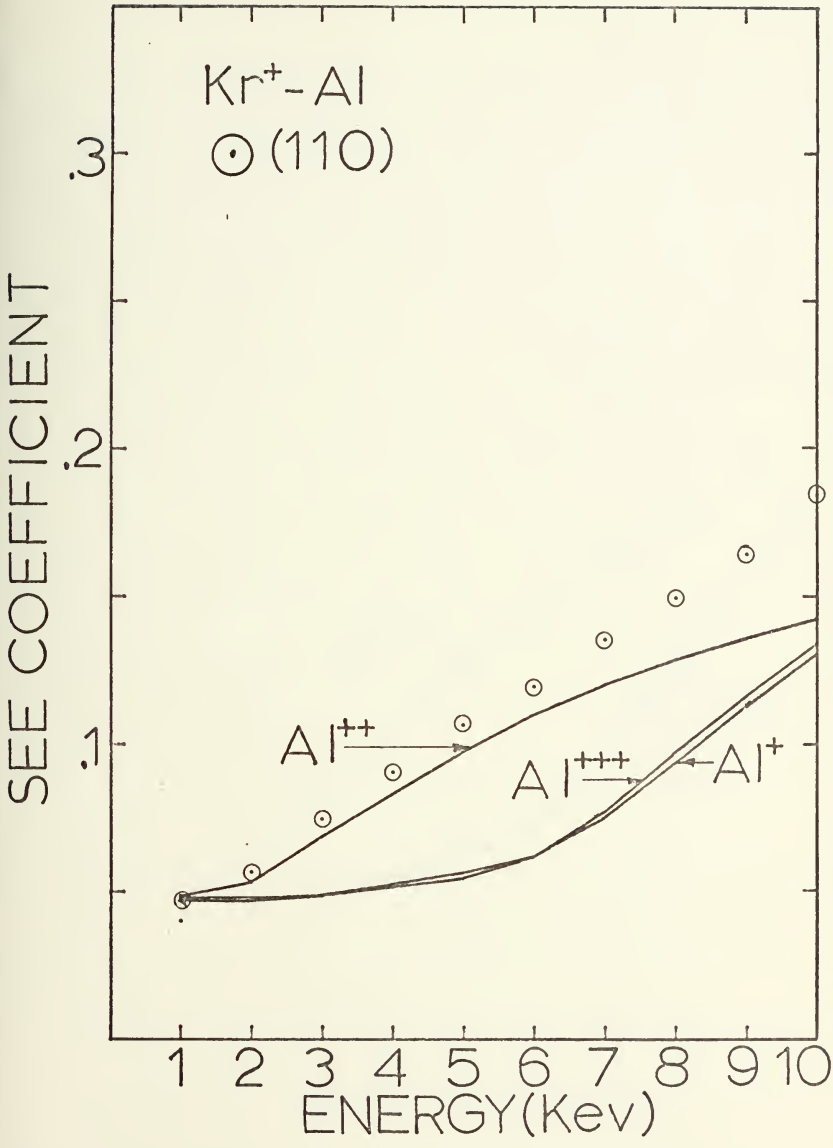

Figure 48. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Kr^{+} - Al system.

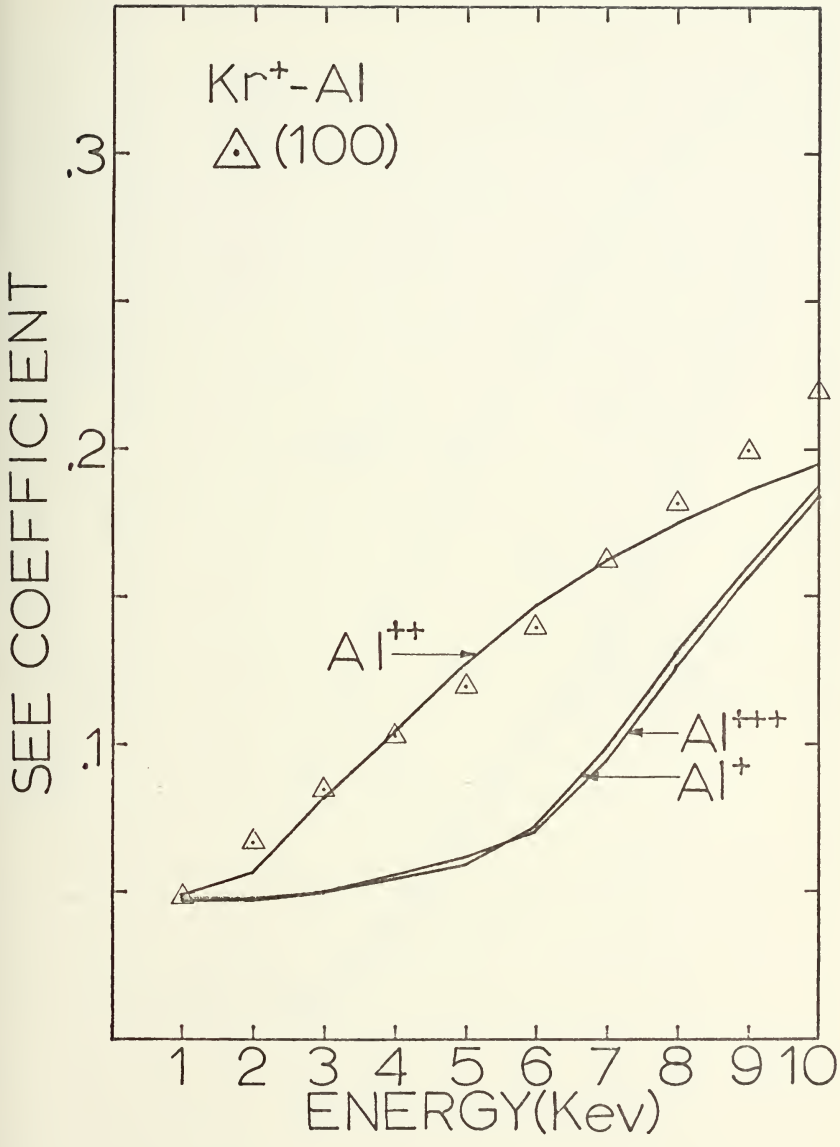

Figure 49. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Kr^+ - Al system.

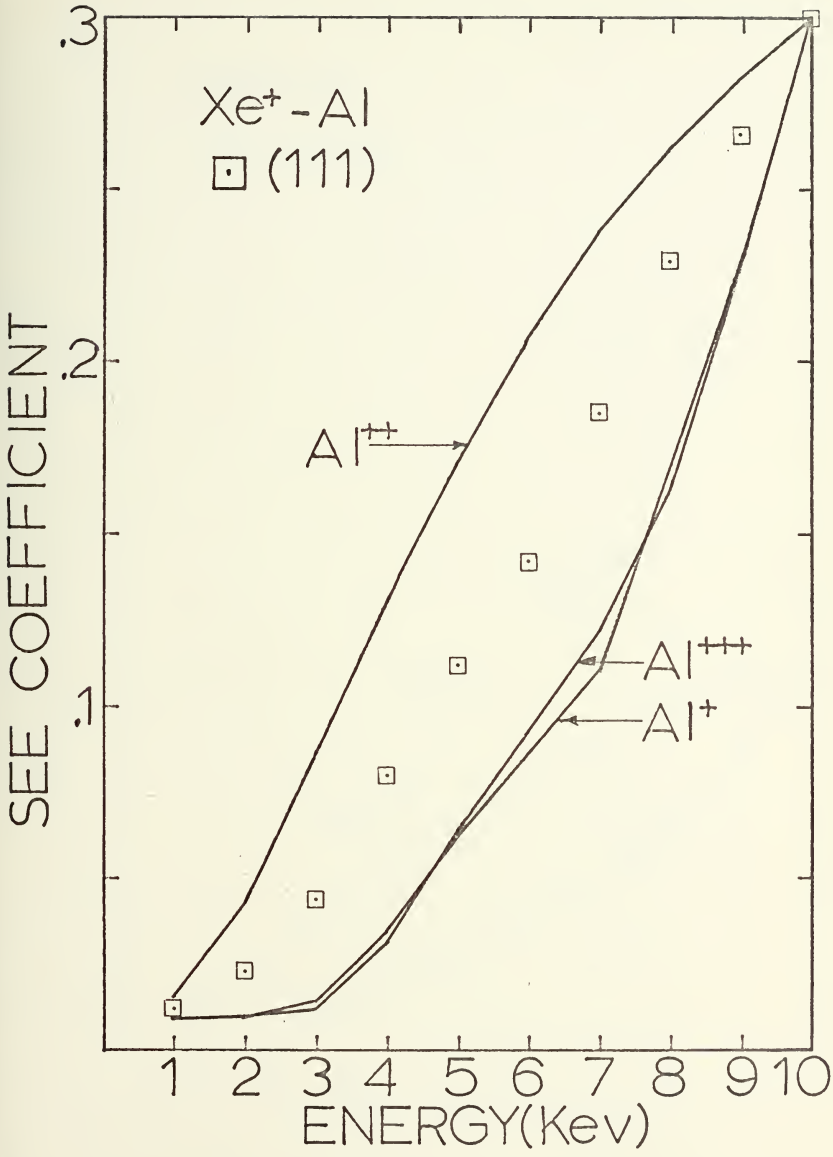

Figure 50. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Xe^{+} - Al system.

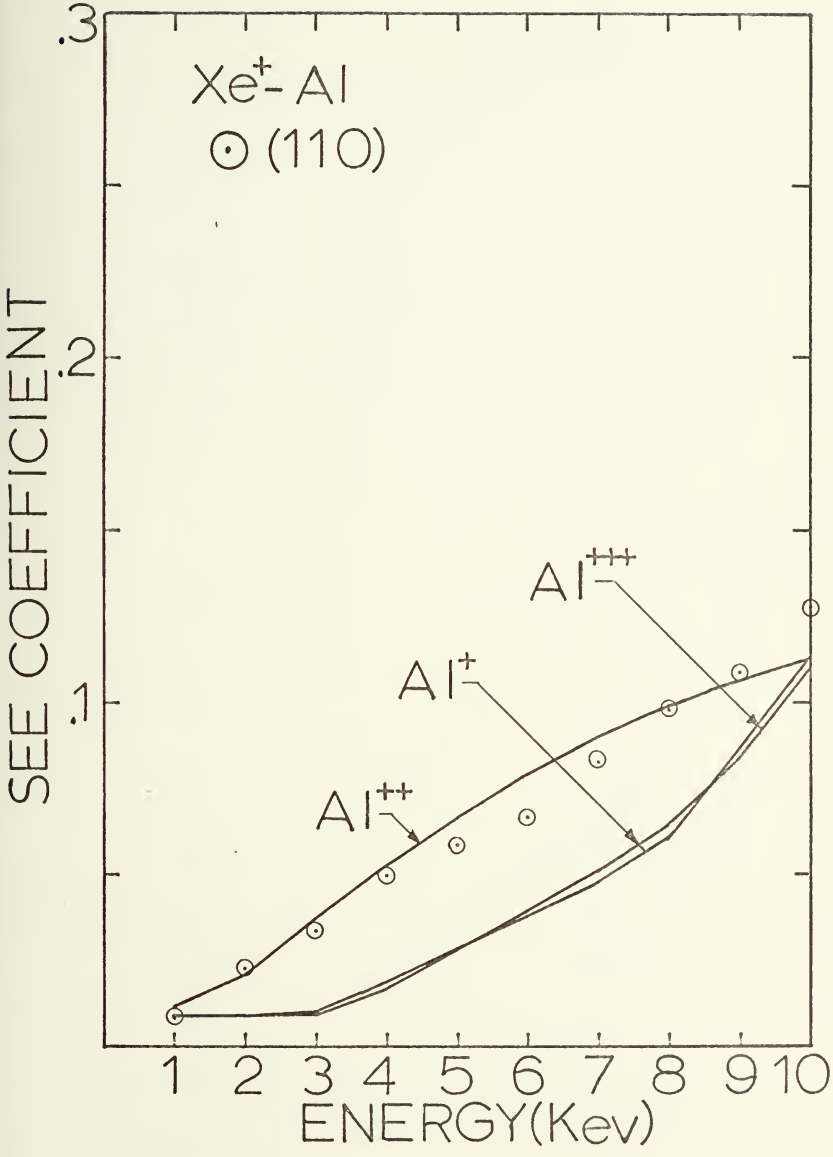

Figure 51. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Xe^+ - Al system.

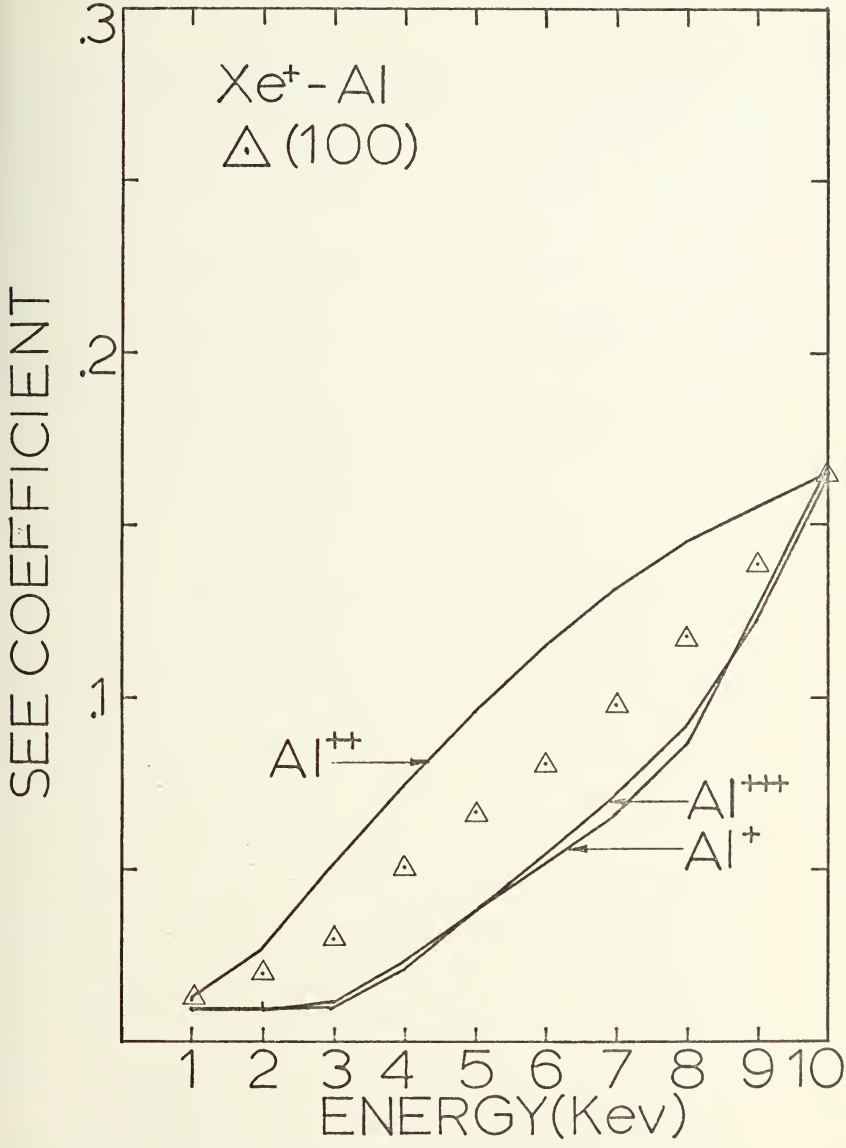

Figure 52. Effect of varying target atom ionization in the HCM model on secondary electron emission from the Xe^+ - Al system.

the bombardment of potassium chloride by argon and neon ions normally incident on the (100), (110) and (111) faces of the single crystal. These two cases are discussed in detail below.

1. Potassium-Chloride Bombarded by Ar Ions

The calculations of the SEE coefficient for alkali-halide single crystals present a theoretical problem that was not addressed when the metal target results were presented. Specifically, the alkali-halide crystals in question have lattice structures comprised of two different atoms arranged in a similar fashion, but displaced in space by a distance (1/2, 1/2, 1/2). Because of this, the standard FCC distribution of impact parameters does not work in the alkali-halide case and must be replaced by a distribution representative of the normal impact of an ion with the target surface. The representative areas and distribution of impact parameters are chosen in a manner similar to that for the metal case, but are weighted to include preferential impact with the larger of the two ion cores in the lattice. The representative areas and distribution of impact parameters are shown in Figures 53 through 57.

The results for KCl bombarded by Ar^+ are shown in Figure 58. Experimentally, it was found that the SEE

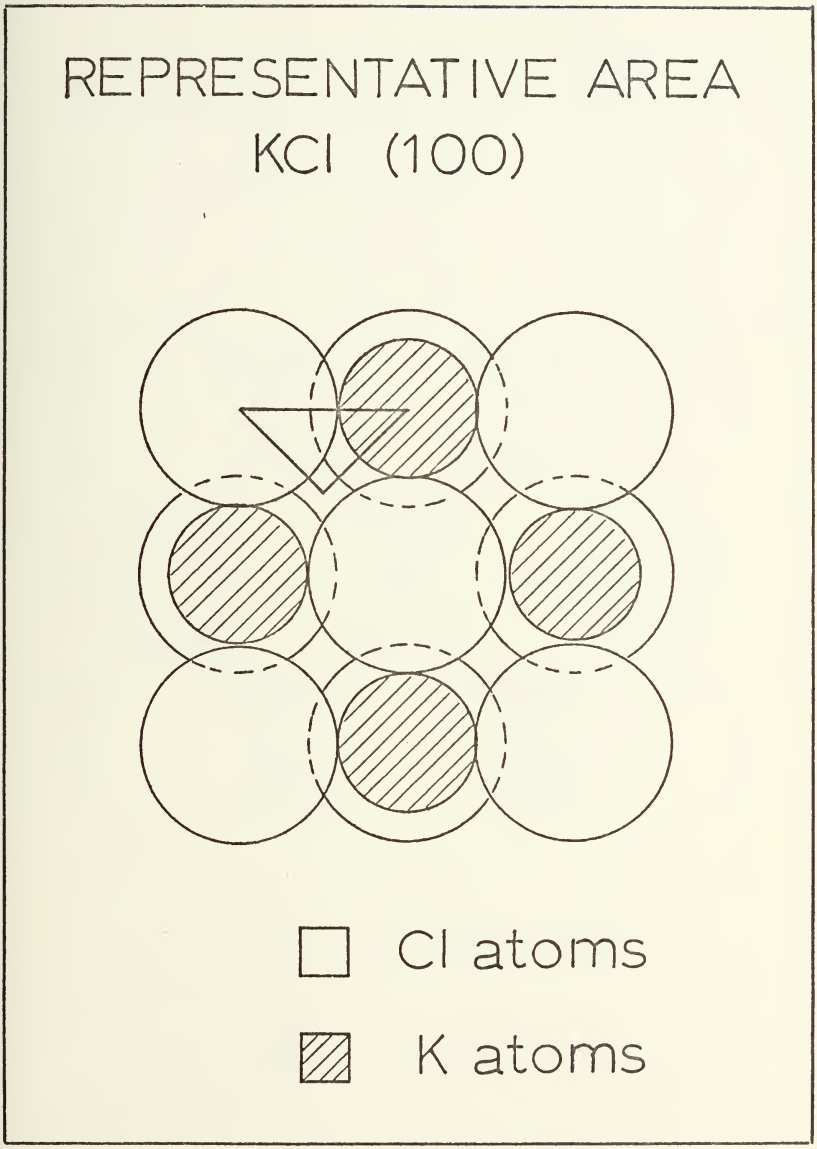

Figure 53. Representative area KCl (100).

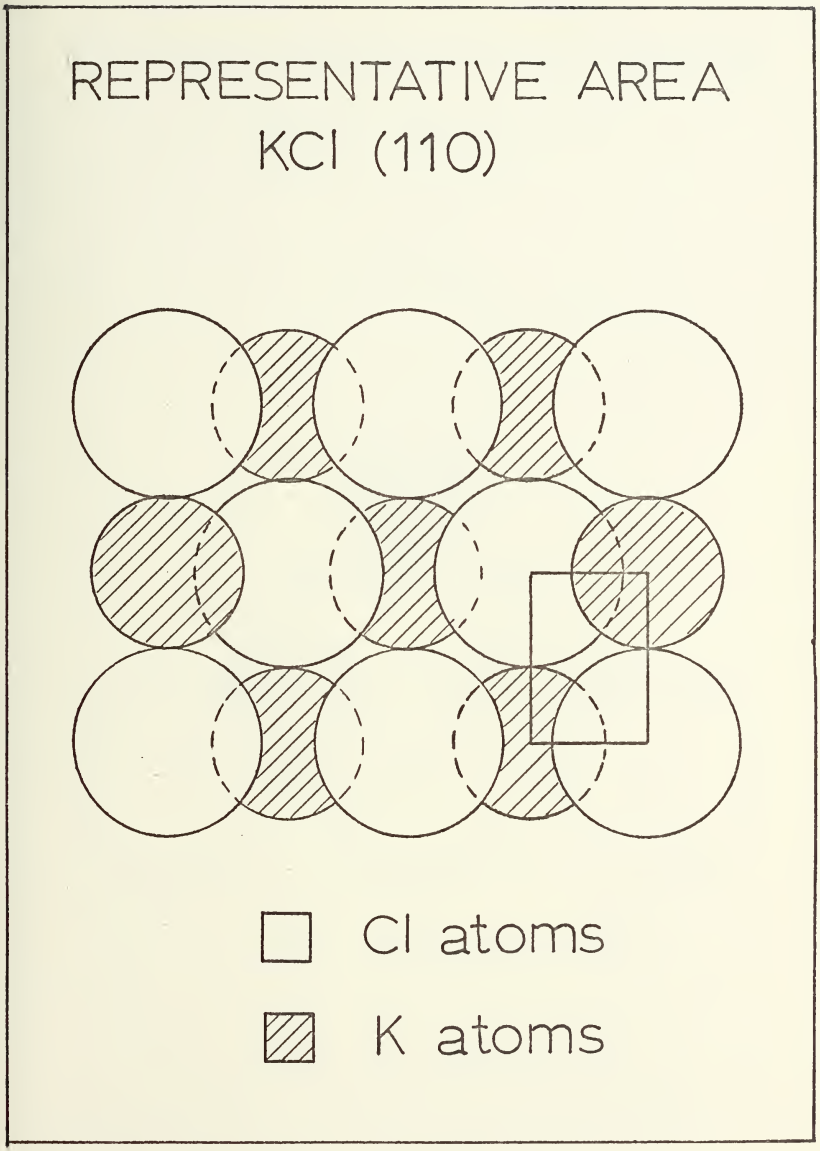

Figure 54. Representative area KCl (110).

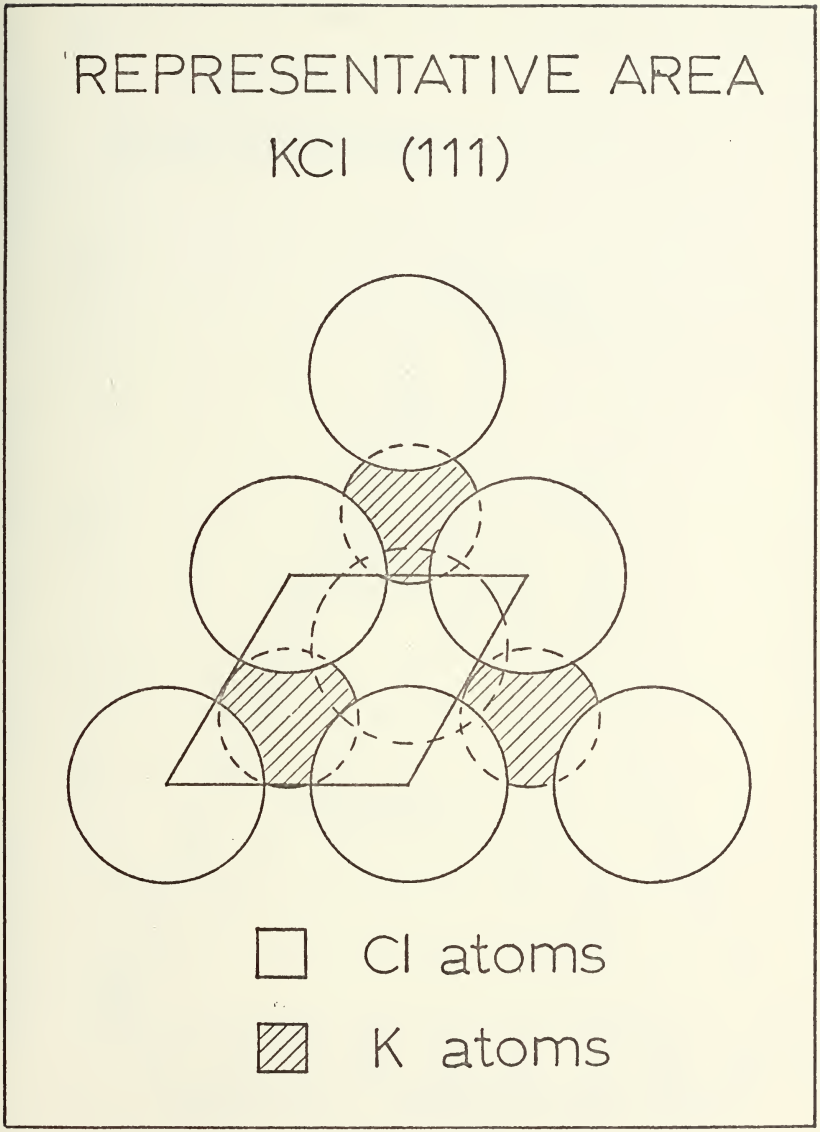

Figure 55. Representative area KCl (111).

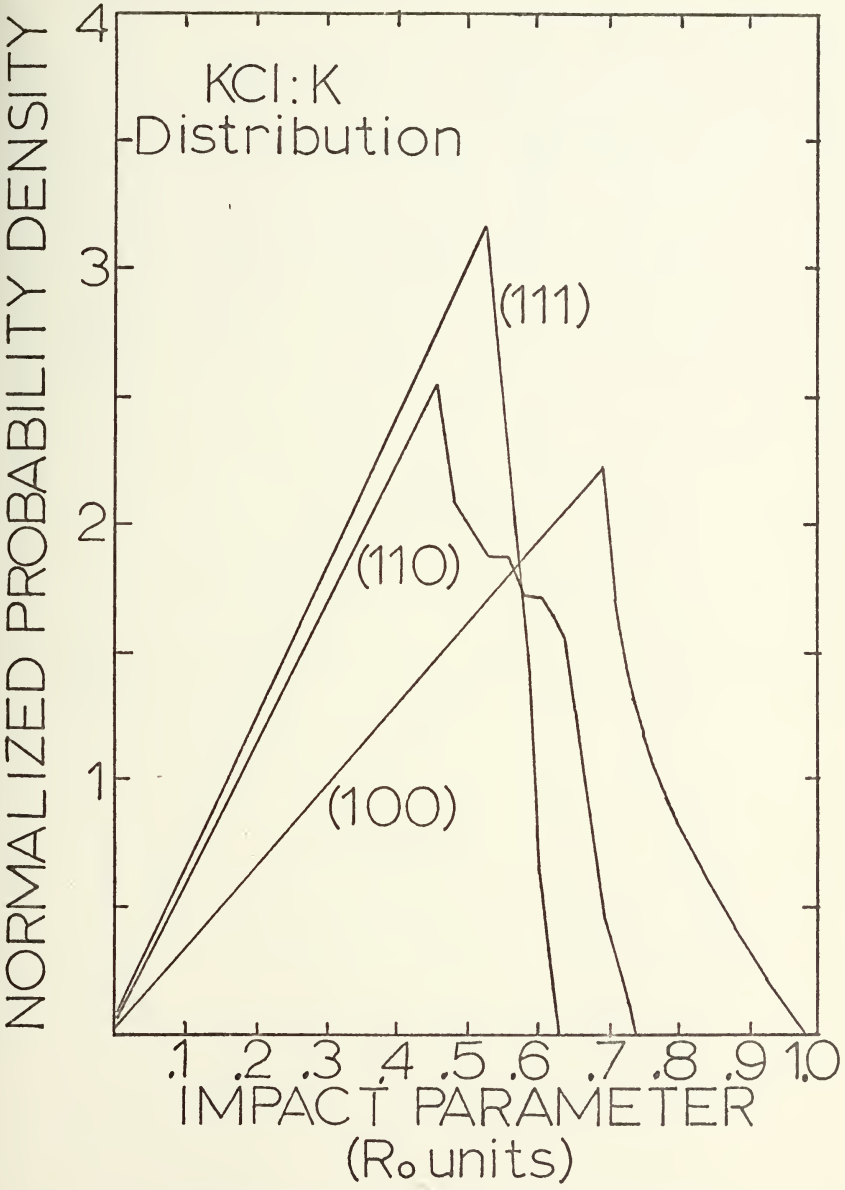

Figure 56. Potassium distribution of impact parameters in KCl.

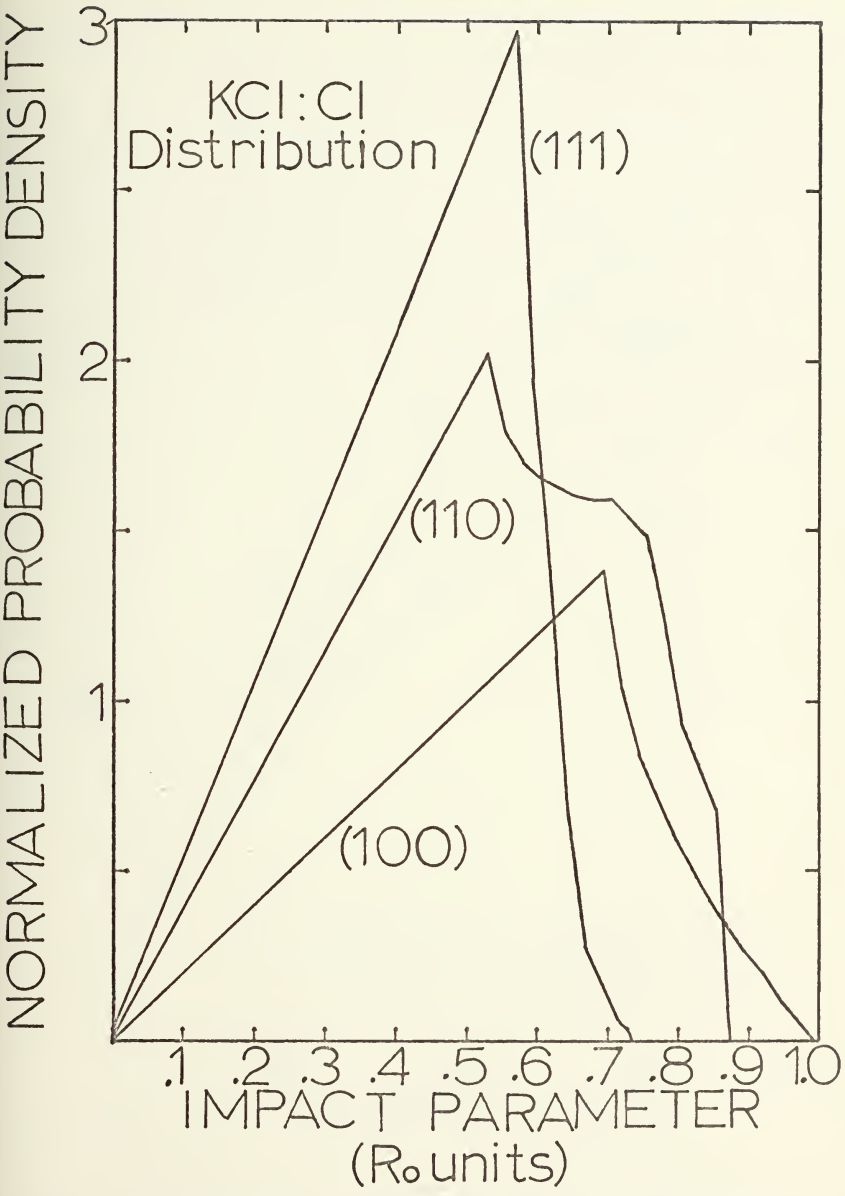

Figure 57. Chlorine distribution of impact parameters in KCl.

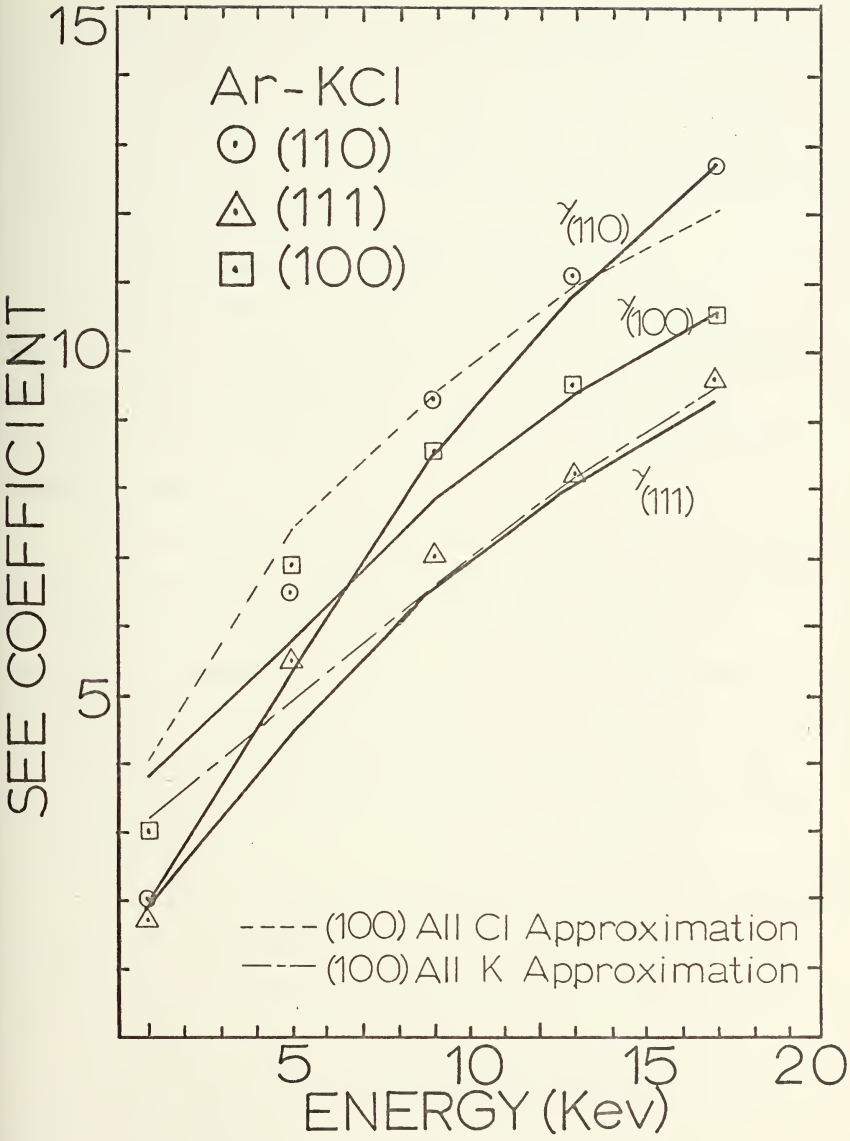

Figure 58. SEE coefficient as a function of energy for KCl bombarded by Ar^+ ions.

coefficient for the (100) face crossed that of the (110) face in the five to six Kev region. This behavior, as well as that for the (111) and (110) faces, is predicted by the HCM modified model. A PSE contribution is evident but has not been investigated.

2. Potassium-Chloride Bombarded by Ne Ions

In the case of KCl bombarded by Ne^+, the HCM modified model predicts a crossing of the (100) and (110) surfaces' SEE coefficients as a function of energy at approximately five Kev. Such a behavior is not confirmed experimentally.

In an attempt to explain this anomaly, two theories arose. First, such a behavior can be explained, if the KCl crystal tends to cleave on the (100) face with all the chlorine or potassium atoms up. Second, the crossing behavior might be due to preferential sputtering by the primary ion of one of the two types of atoms comprising the (100) face, leaving a surface that contains either all potassiums or all chlorines.

In the first case, the crystal structure of the (100) face should be the same for both Ar^+ and Ne^+ bombardment, as long as preferential sputtering does not occur. Hence, SEE from this face should be due to the bombardment of either pure chlorine or pure potassium, whichever is left in the "up" position.

In the second case, however, preferential sputtering of chlorine atoms by Ar^+ is the case most likely to occur,

since both the ion and target atom are of comparable mass. In this situation, preferential sputtering would affect the Ar^+ - KCl system more than it would the Ne^+ - KCl system. Since the Ar^+ - KCl system's SEE coefficient as a function of energy is accurately predicted for all surfaces examined, it appears that sputtering is not directly responsible for the results that are obtained from either system.

The effect of an all-potassium or all-chlorine approximation to the KCl (100) surface on the SEE coefficient as a function of energy and primary ion type is shown graphically in Figures 58 and 59.

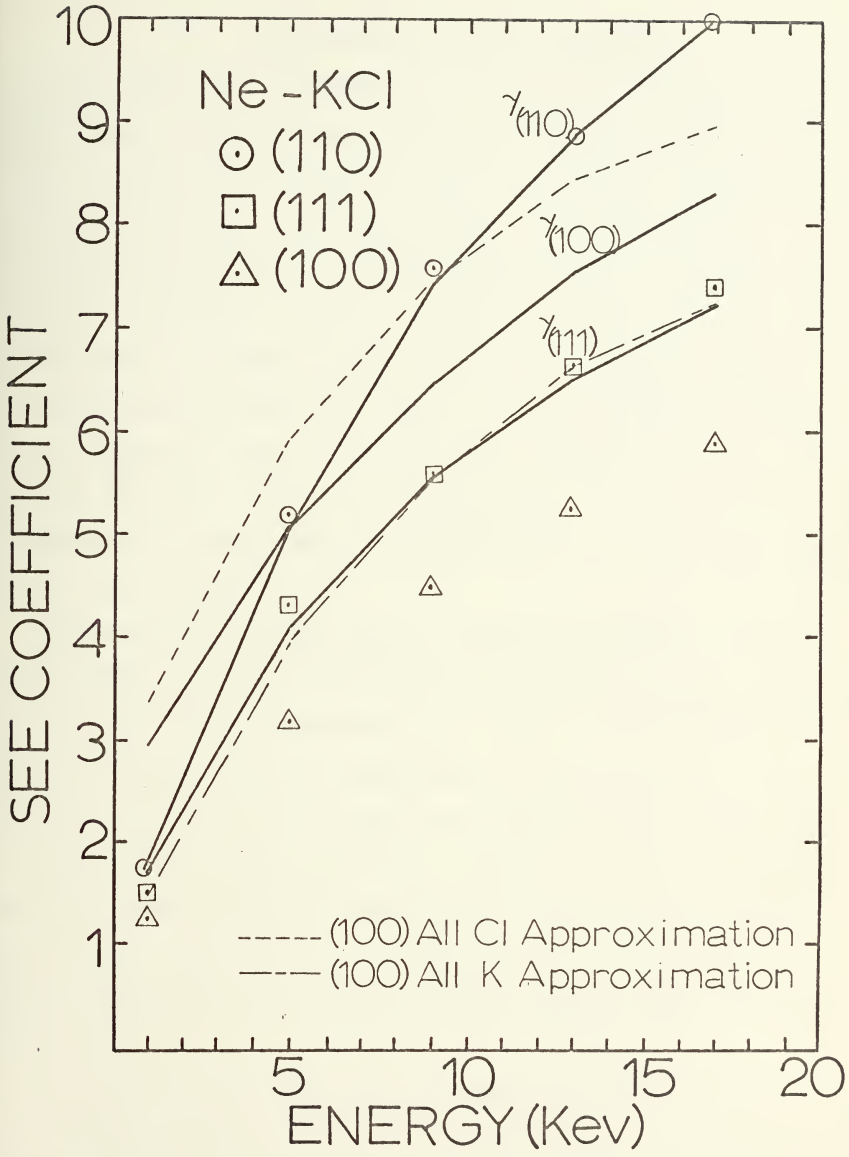

Figure 59. SEE coefficient as a function of energy for KCl bombarded by Ne^+ ions.

VIII. CONCLUSIONS AND RECOMMENDATIONS

This thesis has attempted to predict the behavior of the coefficient of ion electron emission for various primary ion-target combinations using the Harrison, Carlston and Magnuson theory of secondary electron emission. Three aspects of secondary electron emission were investigated, including angularly dependent secondary electron emission from the (100) face of a copper single crystal rotated about <$\bar{1}$10>, secondary electron emission from Ar, Ne, Kr and Xe ions normally incident on the (100), (110) and (111) faces of Cu, Ag, Mo and Al single crystals, and secondary electron emission from Ar and Ne ions normally incident on the (100), (110) and (111) faces of KCl.

According to the HCM theory, angularly dependent results do not demonstrate the non-monotonic dependence on the angle of incidence found experimentally. Even so, the HCM theory does accurately model the dependence of the SEE coefficient of angle of incidence for inert gas ions normally incident on a polycrystalline metal surface. For this reason, it appears that the single collision model is not sophisticated enough and further modification must be made to it, if secondary electron emission from rotated, single-crystal faces is to be predicted.

In the case of metal targets bombarded by inert gas ions, it was found that the SEE coefficient as a function of energy, predicted by the modified HCM movel, deviated from that experimentally obtained. This was contrasted with the results obtained using HCM's original model which yielded

reasonable results in almost all cases investigated. Since the modifications presented here were refinements to the original HCM model, it was hoped the results obtained would more accurately represent the secondary electron mechanism. For this reason, the difference between the SEE coefficient obtained here and the experimental result was identified as the potential secondary electron emission component operating at higher energies. Such a hypothesis is substantiated by experiment [1]. Analysis showed that the potential component in general rose to a peak and then decreased at higher energies. Furthermore, this component of secondary emission seemed to demonstrate behavior that could possibly be attributed to primary ion type as well as the face of the crystal being bombarded. The reason for this behavior was not positively identified, but the PSE process appears to be more complicated than was originally thought.

In the case of potassium-chloride bombarded by Ar ions, the HCM model fairly accurately predicted the SEE coefficient in the zero to 20 Kev energy range for all faces examined. On the other hand, potassium-chloride bombarded by Ne ions demonstrated a crossing of the SEE coefficient for the (100) and (110) faces as a function of energy which was not predicted experimentally. Two hypotheses were proposed that might possibly explain this behavior. The first hypothesis proposes that KCl cleaves with either all the potassium atoms or all the chlorine atoms up, essentially presenting a uniform layer of pure potassium or chlorine to the bombarding ion

beam. This hypothesis slightly improved the SEE coefficient for the Ne^+ KCl (100) surface, but adversely affected the results obtained for the Ar^+ - KCl system. The second hypothesis assumes that the (100) surface of KCl might demonstrate preferential sputtering. However, if this were the case, preferential sputtering should have been most evident in the Ar^+ - KCl system, because of the comparable mass of Ar and Cl. Since this system demonstrated the correct behavior without invoking the preferential sputtering assumption, it was surmised that preferential sputtering did not play an important role in the SEE process from the KCl (100) surface.

In all cases tested in the present investigation, the SEE coefficient as a function of energy tended to become a better approximation to the experimental results at higher energies. For this reason, it is recommended that primary ion-target atom combinations be run for primary ion energies between ten and 20 Kev. If in fact the potential component of secondary electron emission is real in this energy range, it should reach some constant value as primary ion energy is increased. Furthermore, because results obtained using the modified HCM model are dependent on the ion core configuration of the target atoms, it is recommended that more work be done in testing the influence of ion-target atom core ionization on secondary electron emission. Typically, for secondary electron emission from elements such as Cu and Ag, which appear in column I of the periodic table, the

ion core electron configuration is uniquely determined by considerations of the atomic valence, but the effect of the electronic structure of the ion core upon KSE for Mo and Al needs more investigation.

APPENDIX A

COMPUTER PROGRAMS

In this appendix, the parameters that appear in the computer programs are presented and explained. Variables that appear in the data input as constants are stated as such. A pictorial representation of how these data are entered into the programs is shown in Figures 12 - 16.

A. HERMAN SKILLMAN RADIAL ELECTRON DENSITY PROGRAM

CARD #	NAME	FORMAT	DESCRIPTION
1	HEADER CARD - CONTAINS 80 CHARACTERS OF INFORMATION DESCRIBING THE CASE TO BE RUN		
2	KEY	(I4)	SEE Reference ( ), 0
2	TOL	(F8.6)	" , 000001
2	THRESH	(I4)	" , 521
2	MESH	(I4)	" , 1
2	IPRATT	(I4)	" , 40
2	MAXIT	(I4)	" , 0
2	NOCOPY	(I4)	" , 0
2	KUT	(I4)	" , 0
3-A*	RU2(I)	(IPE15.7, IP4E14.7)	Normalized self-consistent potential as a function of X. Taken directly from Reference 16. This is a "starter" for generating the wavefunctions for the atom under investigation.
B	Z	(F4.0)	Atomic number of atom in question
B	NCORES	(I4)	No. of shells of atom in question
B	NVALES	(I4)	0
B	ION	(I4)	Degree of ionization of atom in question
C	NNLZ(I)	(I4)	n,l,m quantum no. for shells
C	WWNL(I)	(F4.0)	No. electrons in shell
C	EE(I)	(F8.4)	Trial eigenvalue for each shell, taken from Reference 16.

B. POTENTIAL PROGRAM

CARD #	NAME	FORMAT	DESCRIPTION
1	INUC	(I2)	0
1	KSTEP	(I3)	10
1	AZ	(F3.0)	Atomic no. of the first atom following the header card below.
1	AI	(F2.0)	Ionization of the first atom following the header card.
1	BZ	(F3.0)	Atomic no. of the second atom following the header card.
1	BI	(F2.0)	Ionization of the second atom following the header card.
1	DM	(F2.0)	5
1	RM	(F2.0)	5
1	RTEST	(F2.0)	5
1	DD	(F5.1)	.020
1	FRR	(F5.1)	1.20
1	DRS	(F5.1)	.010
1	IPN	(I4)	1
2	HEADER CARD - CONTAINS 30 CHARACTERS OF INFORMATION DESCRIBING THE CASE TO BE RUN		
3	OUTPUT FROM ELECTRON DENSITY PROGRAM WITH FIRST CARD REMOVED CORRESPONDING TO THE ATOM DESCRIBED BY AZ AND AI ABOVE		
4	OUTPUT FROM ELECTRON DENSITY PROGRAM WITH FIRST CARD REMOVED CORRESPONDING TO THE ATOM DESCRIBED BY BZ AND BI ABOVE		

C. DISTRIBUTION OF IMPACT PARAMETERS PROGRAM

CARD #	NAME	FORMAT	DESCRIPTION
1	HEADER CARD - 80 CHARACTERS OF INFORMATION DESCRIBING THE CASE TO BE RUN		
2	ICODE	(I3)	1, if representative area is a rectangle 2, if representative area is a triangle
2	A	(F10.4)	Height of representative area in Ro units.
2	B	(F10.4)	Length of representative area in Ro units.
2	INUMBER	(I3)	No. of atoms in representative area.

C. DISTRIBUTION OF IMPACT PARAMETERS PROGRAM (Continued)

CARD #	NAME	FORMAT	DESCRIPTION
3	LARGE(I)	(I2)	Logical array that indicates if any particular atom is larger than the other, i.e., Cl in KCl. 1, yes. 2, no. If yes the distribution is skewed to indicate preferential collision with the larger atom.
4	SCALEF	(F10.4)	1.0
4	RNA	(F10.4)	Ionic radius of smaller of two atoms.
4	RCL	(F10.4)	Ionic radius of larger of two atoms--Both RNA and RCL can be set to anything if atoms are both the same size.
5-7	A5(I,J)	(3F10.4)	An array that contains the (x,y) vertices of a triangular representative area in Ro units. If the area is not triangular, they can be set to anything.
8-11	A6(I,J)	(3F10.4)	An array that contains the (x,y,z) position of atoms in the representative area in Ro units. I runs from 1 to INUMBR, J runs from 1 to 3.
12	PHI	(F10.4)	Angle in radians x'-axis makes with x-axis.
12	XR	(F10.4)	(x) position of (x',y') origin.
12	YR	(F10.4)	(y) position of (x',y') origin.
12	ALPHA	(F10.4)	Angle in radians the representative area is rotated through.
12	RMAX	(F10.4)	Maximum impact parameter expected. The no. 250 is usually sufficient.

D. NUMERICAL INTERPOLATION PROGRAM

CARD #	NAME	FORMAT	DESCRIPTION
1	NPOINT	(I4)	No. points from the distribution of impact parameters program to be smoothed.
1	IFLAG	(I4)	1, indicates written output only. 2, indicates written output, card output and graphical output desired.
2	HEADER CARD - 46 CHARACTERS TO BE OUTPUT WITH GRAPHS		
3	HEADER CARD - 46 CHARACTERS TO BE OUTPUT WITH GRAPHS		
4	OUTPUT FROM DISTRIBUTION OF IMPACT PARAMETERS PROGRAM WITH ALL "NEW ATOM" CARDS REMOVED		

E. KSE PROGRAM

CARD #	NAME	FORMAT	DESCRIPTION
1	LCRYST	(A4)	Crystal type "FCC"/"BCC"
1	LTPE	(I2)	1
1	BMAX(I)	(3F6.4)	Maximum impact parameter in Ro units for each face.
1	PUD(I)	(3F6.4)	R_A for each face in Ro units.
1	ARO(I)	(3F6.4)	No. atoms per representative area in Ro units, for each face.
1	LM(I)	(313)	Total number of points in each distribution.
1	KM	(I4)	250
1	FACL	(F7.4)	$(2)^{1/2}/4$ for FCC, $(3)^{1/2}/4$ for BCC.
2-A	FLP(I)	(20I4)	Distribution of impact parameters from Interpolation Program.
B	IH1	80A1	80 characters of information.
C	IH3	19A4	76 characters of information from first card of output from Potential Program.
C	KMR	(I4)	250
D	APSI(I)	10F8.5	Wave functions from the Potential program, Atom A.
D	BPSI(I)	10F8.5	Wave functions from the Potential program, Atom B.

E. KSE PROGRAM (Continued)

CARD #	NAME	FORMAT	DESCRIPTION
E	V(I)	5F12.5	Potential between atoms A and B from the Potential Program.
F	EA(I)	8F8.4	Spectroscopic ionization potentials, numbers 11 to 18.
F+1	IAH	4A4	16 characters of accounting information.
F+1	EA(I)	10F8.4	Spectroscopic ionization potentials, numbers 1 to 10.
F+2	JFIT	I10	No. of values to which results are fit.
G	PSE(I)	(F5.3)	γ_{PSE} experimental for curve being fit.
G	FIT(J)	(F5.4)	γ experimental for (111) face at 10 Kev.
H	ZB	F4.0	Atomic no. for atom A.
H	ZT	F4.0	Atomic No. for atom B.
H	BMAS	F8.4	Atomic weight for atom A.
H	TMAS	F8.4	Atomic weight for atom B.
H	EOS	F8.0	Energy in Kev at which results are to start.
H	DEO	F3.0	Energy step in Kev.
H	KEOM	F3.0	Energy in Kev at which results are to end.
H	AO	F7.3	Lattice constant in angstroms.
H	LSKIP	I3	1
H	NM	I3	15
H	RES	F3.0	50
H	DRE	F3.0	50
H	REM	F5.0	5000
H	IH2	4A4	Accounting data.

*indicates that the actual card number varies from run to run and has been replaced by a letter to indicate the order in which the cards are arranged.

```
// EXEC FORTCLG,REGION.GO=150K
//FORT.SYSIN DD *
C
C      HARTREE-FOCK-SLATER SELF-CONSISTENT ATOMIC FIELD PROGRAM
C      ORIGINALLY WRITTEN BY SHERWOOD SKILLMAN
C      RCA LABORATORIES, PRINCETON NEW JERSEY, SPRING 1961
C      MODIFIED BY FRANK HERMAN,SUMMER 1961
C      FURTHER MODIFIED BY RICHARD KORTUM, LOCKHEED RESEARCH
C      LABORATORIES, PALO ALTO, CALIFORNIA, SUMMER 1962
C      THE PRESENT FORM WAS WRITTEN BY D.E. HARRISON, JR. FOR
C      USE ON THE IBM/360 AT THE NAVAL POSTGRADUATE SCHOOL,
C      MONTEREY, CA. 93940
C
       COMMON/COM1/V(521),R(521),RU(521),RU2(521),RU3(521),X(521),
      2  XI(521),XJ(521),RSCORE(521),RSATOM(521),RSVALE(521),
      3  RUINL1(521),RUINL2(521),RUFNL1(521),RUFNL2(521),RUEXCH(521),
      4  XNUM(521),DENM(521),SNLO(521),CC(521),RR(521),
      5  NNLZ(24),WWNL(24),NKKK(24),EE(24),A(4,5),SNL(24,521)
       START=0.01*ITIME(XX)
       DO 9500 I=1,521
       V(I)=0.0
       R(I)=0.0
       RU(I)=0.0
       RU2(I)=0.0
       RU3(I)=0.0
       X(I)=0.0
       XI(I)=0.0
       RR(I)=0.0
       XJ(I)=0.0
       RSCORE(I)=0.0
       RSATOM(I)=0.0
       RSVALE(I)=0.0
       RUINL1(I)=0.0
       RUINL2(I)=0.0
       RUFNL1(I)=0.0
       RUFNL2(I)=0.0
       RUEXCH(I)=0.0
       XNUM(I)=0.0
       DENM(I)=0.0
       SNLO(I)=0.0
 9500  CC(I)=0.0
       DO 9510 I=1,24
       NNLZ(I)=0.0
       WWNL(I)=0.0
       NKKK(I)=0.0
 9510  EE(I)=0.0
 9000  FORMAT (72H
      1                                    )
```

```
9010 FORMAT(F8.5,9F7.5)
9020 FORMAT (I4,1P3E14.7,I4,1PE14.7)
9030 FORMAT(F4.0,3I4)
9040 FORMAT(9F8.8)
9050 FORMAT(6H WWW =F4.0,6H ZZZ= F4.0,6H   Z =F4.0,11H   NCORES = I4,
   1 11H   NVALES = I4,11H   NCSPVS= I4/25H CONTROL CARDS INCORRECT. )
9060 FORMAT(6F5.2,F10.3)
9070 FORMAT(I4,F4.0,F8.4)
9080 FORMAT(I7,F7.0,1PE14.7,0P2(I6,F9.3))
9090 FORMAT(6(I5,1PE14.7))
9100 FORMAT(1PE15.7,1P4E14.7)
9110 FORMAT(10H  NCARDS= I4, 10H  MCARDS = I4)
9120 FORMAT(I4,2F8.6,5I4)
9130 FORMAT(2F4.0,2F7.3)
9140 FORMAT(6H ZZ1= F4.0,8H   ZZ2= F4.0,10H   BETA1= F7.3,
   1 10H   BETA2= F7.3)
9150 FORMAT(7H  KEY = I4)
9160 FORMAT  (6H  ITER,7X,1HZ,4X5HDEL A,7X,30HI(DEL)  I(CUT)  X
   1(CUT)  )
9170 FORMAT(I4,1P3E14.7,I4,1PE14.7,8X,1HZ,I3,I4)
9180 FORMAT(F4.0,3I4,56X,1HZ,I3,I4)
9190 FORMAT(1PE15.7,1P4E14.7,1X,1HZ,I3,I4)
9200 FORMAT (1PE15.7,57X,1HZ,I3,I4)
9210 FORMAT (27HOSTARTING POTENTIALS AND Z=,F4.0,9H IN ERROR,2F4.0)
9220 FORMAT  (40H1I,X,RU3,RUINL1,RUFNL1,RUINL2,RUFNL2,RU    )
9230 FORMAT  (I8,F10.4,1P6E16.7)
     NFILES =0
  10 READ(5,9000)
     WRITE(6,9000)
     READ(5,9120) KEY,TOL,THRESH,MESH,IPRATT,MAXIT,NOCOPY,KUT
     NCARDS=90
     WRITE(6,9150) KEY
     IF(MAXIT) 20,20,30
  20 MAXIT=20
  30 NBLOCK = MESH/40
     I=1
     X(I)=0.0
     R(I)=0.0
     DELTAX=0.0025
     THIRD=1.0/3.0
     R8=1.0/8.0
     R24=1.0/24.0
     R32=1.0/32.0
     R315=1.0/315.82734
     DO 40 J=1,NBLOCK
     DO 35 K=1,40
     I=I+1
  35 X(I)=X(I-1)+DELTAX
```

```
 40 DELTAX=DELTAX+DELTAX
    IF(KEY-1) 60,70,50
 50 READ (5,9100) (RU2(M) ,M=1,441)
    READ (5,9100) (RU3(M) ,M=1,441)
    ZE2=-0.5*RU2(1)
    ZE3=-0.5*RU3(1)
    GO TO 100
 60 READ (5,9010) (RU2(M) ,M=1,437,4)
    GO TO 100
 70 READ (5,9100) (RU3(M),M=1,441)
    ZE3=-0.5*RU3(1)
100  READ(5,9030) Z,NCORES,NVALES,ION
     IF (Z) 9999,10,110
110   NFILES =NFILES+1
    IZ=Z
    TZ=Z+Z
    NCSPVS=NCORES+NVALES
    C=0.88534138/Z**THIRD
    TWOION=ION+ION
    ZZZ=ION+1
    TWOZZZ = ZZZ+ZZZ
    DO 120 I=2,MESH
    R(I)=C*X(I)
120 RR(I)=1.0/R(I)
     READ(5,9070) (NNLZ(I),WWNL(I),EE(I),I=1,NCSPVS)
    WWW=0.0
    DO 130 I=1,NCSPVS
130 WWW=WWW+WWNL(I)
    IF(ABS(Z+1.0-WWW-ZZZ)-0.001) 150,140,140
140 WRITE(6,9050) WWW,ZZZ,Z,NCORES,NVALES,NCSPVS
    GO TO 9999
150 IF (KEY-1) 300,400,200
200 IF(ABS(ZE3-ZE2-Z+ZE3)-0.001) 220,220,210
210 WRITE(6,9210) Z,ZE2,ZE3
    GO TO 9999
220 DO 250 I=1,441
250 RU(I) =RU3(I)+RU3(I)-RU2(I)
    GO TO 500
300 TWOZ=TZ
    DO 310 I=1,437,4
310 RU(I)=-RU2(I)*TWOZ
    RU(441)=RU(437)
    RU(445)=RU(437)
    M=9
    DO 350 I=1,437,4
    M=M-1
    IF(M) 320,330,330
320 RU(I+1)=(22.0*RU(I)+11.0*RU(I+4)-RU(I+8))*R32
```

```
      RU(I+2)=(10.0*RU(I)+15.0*RU(I+4)-RU(I+8))*R24
      RU(I+3)=( 6.0*RU(I)+27.0*RU(I+4)-RU(I+8))*R32
      M=9
      GO TO 350
  330 RU(I+1)=(21.0*RU(I)+14.0*RU(I+4)-3.0*RU(I+8))*R32
      RU(I+2)=( 3.0*RU(I)+ 6.0*RU(I+4)-    RU(I+8))*R8
      RU(I+3)=( 5.0*RU(I)+30.0*RU(I+4)-3.0*RU(I+8))*R32
  350 CONTINUE
      GO TO 500
  400 IF(ABS(ZE3-Z)-0.001)  410,410,430
  410 DO 420 I=1,441
  420 RU(I)=RU3(I)
      GO TO 500
  430 ZOZ=Z/ZE3
      DO 440 I=1,441
  440 RU(I)=RU3(I)*ZOZ
  500 V(1)=-9.9E35
      M=MIN0(441,MESH)
      IF(KUT)  600,700,600
  600 DO 610 I=1,M
  610 V(I)=RU(I)*RR(I)
      IF(MESH-M) 620,620,640
  620 DO 630 I=442,MESH
  630 V(I)=-TWOICN*RR(I)
  640 LIMIT=M
      ICUT=MESH
      IC=MESH
      GO TO 900
  700 ICUT=0
      DO 750 I=2,M
      IF (ICUT) 710,710,730
  710  IF( TWOZZZ+RU(I)) 740,740,720
  720 ICUT =I
  730 V(I)=-TWOZZZ*RR(I)
      GO TO 750
  740 V(I)=RU(I)*RR(I)
  750 CONTINUE
      IF (ICUT) 790,790,800
  790  ICUT=M
  800 LIMIT=ICUT
      IF(MESH-M) 900,900,810
  810 DO 850 I=442,MESH
  850 V(I)=-TWOZZZ*RR(I)
  900 DELTA =1000000.
      NITER=0
      NONMOM=3
      IPRSW=0
      WRITE(6,9160)
```

```
1000 MCARDS=90
     IF(MAXIT-NITER) 1100,2000,2000
1100 WRITE(6,9220)
     DO 1500 I=1,MESH,5
     WRITE( 6,9230) I,X(I),RU3(I),RUINL1(I),RUFNL1(I),
    1  RUINL2(I),RUFNL2(I),RU(I)
1500 CONTINUE
     GO TO 100
2000 DO 2010 I=1,MESH
     RSCORE(I)=0.0
2010 RSVALE(I)=0.0
     DO 2500 M=1,NCSPVS
     E=EE(M)
      NN=NNLZ(M)/100
      LAM =NNLZ(M)/10 -10*NN
      XL= LAM
      CALL SCHEQ(Z,E,LAM,NN,KKK,MESH,C,THRESH)
     IF(M-NCORES) 2100,2100,2200
2100 DO 2150 I=1,KKK
     SNL(M,I)=SNLO(I)
2150 RSCORE(I)=RSCORE(I)+WWNL(M)*SNLC(I)*SNLO(I)
     GO TO 2300
2200 DO 2250 I=1,KKK
     SNL(M,I)=SNLO(I)
2250 RSVALE(I)=RSVALE(I)+WWNL(M)*SNLO(I)*SNLO(I)
2300 NKKK(M)=KKK
     MCARDS=MCARDS+2+((KKK-1)/40)*8
2500 EE(M)=E
     DO 2600 I=1,MESH
     RSATOM(I)=RSCORE(I)+RSVALE(I)
2600 RUEXCH(I)= -6.0*(3.0*R(I)*RSATOM(I)*R315)**THIRD
     A1=0.0
     ASUM=0.0
     B1=0.0
     BSUM=0.0
     H=0.0025*C
     I=1
     XI(1)=0.0
     XJ(1)=0.0
     DO 2620 J=1,NBLOCK
     DO 2610 K=1,40
     I=I+1
     A2=RSATOM(I)*0.5
     A1=A1+A2
     B2=A2*RR(I)
     B1=B1+B2
     XI(I)=ASUM+A1*H
     XJ(I)=BSUM+B1*H
```

```
      A1=A1+A2
2610  B1=B1+B2
      ASUM=XI(I)
      BSUM=XJ(I)
      A1=A2
      B1=B2
2620  F=F+H
      DO 2650 I=1,MESH
      XI(I)=-TZ+2.0*(XI(I)+R(I)*(XJ(MESH)-XJ(I)))
      XJ(I)=XI(I)+RUEXCH(I)
2650  CONTINUE
      DO 2700 I=1,MESH
      RUINL1(I)=RUINL2(I)
      RUFNL1(I)=RUFNL2(I)
      RUINL2(I)=RU(I)
2700  RUFNL2(I)=XJ(I)
      NITER=NITER+1
      PDELTA=DELTA
      DELTA=0.0
      DO 2800 I=1,LIMIT
      SNLO(I)=RU(I)-XJ(I)
      XI(I)=ABS(SNLO(I))
      IF (XI(I)-DELTA) 2800,2800,2750
2750  DELTA=XI(I)
      IDELTA=I
2800  CONTINUE
      WRITE(6,9080) NITER,Z,DELTA,IDELTA,X(IDELTA),ICUT,X(ICUT)
      IF(DELTA-TOL) 4000,3000,3000
3000  IF(IPRSW) 3100,3100,3150
3100  DO 3110 I=2,LIMIT
3110  RU(I)=0.5*(RU(I)+XJ(I))
      IF (MESH-LIMIT)  3140,3140,3120
3120  RUZM=XJ(MESH)
      RATIO =(RUZM-RU(LIMIT))/(RUZM-XJ(LIMIT))
      DO 3130 I=LIMIT,MESH
3130  RU(I)=RUZM-RATIO*(RUZM-XJ(I))
      LIMIT =MESH
3140  IPRSW=IPRATT
      GO TO 3500
3150  IF(NONMON) 3100,3100,3160
3160  IF(PDELTA-DELTA) 3170,3170,3200
3170  NONMON=NONMON-1
      IF(NONMON) 3100,3100,3200
3200  ALPH=0.5
      DO 3300 I=2,ICUT
      XNUM(I)=RUINL1(I)*RUFNL2(I)-RUINL2(I)*RUFNL1(I)
      DENM(I)=RUFNL2(I)-RUFNL1(I)-RUINL2(I)+RUINL1(I)
      IF(ABS(DENM(I)/RUINL2(I))-0.0001)  3210,3210,3220
```

```
3210 ALPH=0.5
     GO TO 3260
3220 ALPH=(XNUM(I)/DENM(I)-RUFNL2(I))/SNLO(I)
     IF(ALPH) 3230,3260,3240
3230 ALPH=0.0
     GO TO 3260
3240 IF(0.5-ALPH) 3250,3260,3260
3250 ALPH=0.5
3260 XI(I)=ALPH
3300 CONTINUE
     IPRSW=IPRSW-1
     IF(KUT) 3340,3310,3340
3310 IC=ICUT+20
     IC1=ICUT+1
     ADEL=0.05*XI(ICUT)
     DO 3320 I=IC1,IC
     XI(I)=XI(I-1)-ADEL
3320 XJ(I)=XI(I)
3340 XJ(1)=0.5
     XJ(2)=XI(2)
     ASUM=XI(2)+XI(3)+XI(4)+XI(5)
     DO 3350 I=3,ICUT
     XJ(I)=ASUM*0.2
3350 ASUM=ASUM-XI(I-2)+XI(I+3)
     IF(KUT) 3360,3360,3380
3360 IC1=IC+1
     DO 3370 I=IC1,MESH
     XJ(I)=0.0
3370 RU(I)=RUFNL2(I)
3380 DO 3390 I=2,IC
3390 RU(I)=RUFNL2(I)+XJ(I)*SNLO(I)
3500 IF(KUT) 3600,3700,3600
3600 ICUT=MESH
     LIMIT=MESH
     DO 3650 I=2,MESH
     VLAST= V(I)
     V(I)=RU(I)*RR(I)
3650 XI(I)=V(I)-VLAST
     GO TO 3900
3700 ICUT =0
     DO 3890 I=2,MESH
      VLAST=V(I)
     IF(ICUT) 3820,3820,3860
3820 IF(TWOZZZ+RU(I)) 3880,3880,3840
3840 ICUT=I
3860 V(I)=-TWOZZZ/R(I)
     GO TO 3890
3880 V(I)=RU(I)*RR(I)
```

```
3890 XI(I)=V(I)-VLAST
3900 XI(1)=0.0
     NCARDS=90
     DO 3990 M=1,NCSPVS
     K=(NKKK(M)-1)/40
     H=0.0025*C
     HH=0.5*H
     ASUM=0.0
     A1=0.0
     I=1
     DO 3960 J=1,K
     DO 3940 L=1,40
     I=I+1
     A2=XI(I)*SNL(M,I)*SNL(M,I)
3940 A1=A1+A2*H
     ASUM=ASUM+A1-A2*HH
     HH=H
     H=H+H
3960 A1=HH*A2
     EE(M)=EE(M)+ASUM
3990 NCARDS=NCARDS+8*K+2
     GO TO 10000
4000 WRITE (6,9110) NCARDS,MCARDS
     NC=1
     WRITE(6,9180) Z, NCORES,NVALES,ICN,IZ,NC
     DO 4190 I=1,441
     IF(TWOION+RUINL2(I)) 4190,4190,4120
4120 DO 4140 M=I,441
4140 RUINL2(M)=-TWOION
     GO TO 4200
4190 CONTINUE
4200 DO 4220 MIN=1,440,5
     MAX=MIN+4
     NC=NC+1
4220 WRITE(6,9190)(RUINL2(M),M=MIN,MAX),IZ,NC
     WRITE(7,9970) Z,ICN
9970 FORMAT(F10.1,I5)
     WRITE(7,9960) (RSATOM(I),I=1,441)
     WRITE(6,9960) (RSATOM(I),I=1,441)
9960 FORMAT(5E15.7)
     NC=NC+1
     WRITE(6,9200) RUINL2(441),IZ,NC
     DO 4400 M=1,NCSPVS
     NLZ=NNLZ(M)
     KKK=NKKK(M)
     XL=NLZ/10-10*(NLZ/100)
     LP=XL+1.0
     DO 4350 I=1,4
```

```
      A(I,1)=1.0
      A(I,2)=R(I+1)
      A(I,3)=R(I+1)*R(I+1)
      A(I,4)=R(I+1)*A(I,3)
4350  A(I,5)=SNL (M,I+1)*RR(I+1)**LP
      CALL CRCSYM (4)
      NC=NC+1
      WRITE(6,9170) NLZ,XL,EE(M),WWNL(M),KKK,A(1,5),IZ,NC
      K1=KKK-1
      DO 4380 MIN=1,K1,5
      NC=NC+1
      MAX=MIN+4
      WRITE(6,9190) (SNL(M,I),I=MIN,MAX),IZ,NC
4380  CONTINUE
      NC=NC+1
      WRITE(6,9200) SNL(M,KKK),IZ,NC
4400  CONTINUE
      IF(KEY-1)  4420,4440,4480
4420  KEY=1
4440  DO 4460 I=1,MESH
4460  RU2(I)=RU(I)
      ZE3=Z
      GO TO 100
4480  DO 4490 I=1,MESH
      RU2(I)=RU3(I)
4490  RU3(I)=RU(I)
      ZE2=ZE3
      ZE3=Z
      GO TO 100
9999  TIME=0.01*ITIME(XX)-START
      STOP
      END


      SUBROUTINE SCHEQ(Z,E,LAM,NN,KKK,MESH,C,THRESH)
      DIMENSION P(5),Q(5),T(5),D(5)
      COMMON/COM1/V(521),R(521),RU(521),RU2(521),RU3(521),X(521),
     2  XI(521),XJ(521),RSCORE(521),RSATOM(521),RSVALE(521),
     3  RUINL1(521),RUINL2(521),RUFNL1(521),RUFNL2(521),RUEXCH(521),
     4  XNUM(521),DENM(521),SNLO(521),GG(521),RF(521),
     5  ANLZ(24),WWNL(24),AKKK(24),EE(24),A(4,5),SNL(24,521)
      MANY = 200
      MOREV=0
      LESSV=0
      EMORE=0.0
      ELESS=0.0
      MORE=0
      LESS=0
```

```
      DE=0.0
      NPRINT=0
      LAMM=LAM-1
      LAMP=LAM+1
      XLP=LAMP
      NDCR=NN-LAMP
      B=LAM*LAMP
       CC=R(2)
      H=CC
      HSQ=H*H
      B3=(V(3)-V(2))/H-Z/HSQ
      Y=F+H
      FLPS=4*LAM+6
      SLPT=6*LAM+12
      ELPT=8*LAM+20
      A1=-Z/XLP
      YSQ=Y*Y
       E1=-Z-Z
      AE1=A1*E1
      AE3=A1*B3
C     RAISE H AND Y TO LAM+1
      HTL=H
      YTL=Y
      IF(LAM) 105,120,100
  105 NSTOP=105
      GO TO 9900
  100 DO 110 I=1,LAM
      HTL=HTL*H
  110 YTL=YTL*Y
  120 H1=HSQ
      BOHS=B/HSQ
      BOH=B1/H
      BTH=B3*H
      BQ3=BOHS+BOH+BTH
      BQ4=0.25*BOHS+0.50*BOH+BTH+BTH
      EPL=8+LAM
      FPL=5+LAM
      XIFC=C*.2170138 9E-4
C     START OUTWARD INTEGRATION
      EG=E
  200 NPRINT=NPRINT+1
      EPS =E-EG
      EG =E
      IF(MANY-NPRINT)  9920,210,210
  210 DO 220 I=1,MESH
  220 SNLO(I)=0.0
      IF(NPRINT-1) 225,300,400
  225 NSTOP=225
```

```
      GO TO 9900
  300 DO 310 I=4,MESH
  310 GG(I)=V(I)+B*RR(I)*RR(I)-E
  315 M=MESH
      DO 330 I=4,MESH
      IF(GG(M)) 320,330,330
  320 IK=M+1
      GO TO 350
  330 M=M-1
C     Q IS EVERYWHERE POSITIVE
      NSTOP=330
      GO TO 9900
  350 IF(MESH-IK) 360,360,430
  360 EPS = GG(MESH-40)
      E = E+EPS
  400 DO 420 I=4,MESH
  420 GG(I) = GG(I)-EPS
      GO TO 315
  430 NCROSS=0
      SIGN=1.0
      F=GG
      Y=F+H
      B2=3.0*Z/H-E+2.0*V(2)-V(3)
      A2=(AB1+B2)/FLPS
      A3=(A2*B1+A1*B2+B3)/SLPT
      A4=(A3*B1+A2*B2+AB3)/ELPT
      P(3)=(1.0+H*(A1+H*(A2+H*(A3+H*A4))))*HTL
      P(4)=(1.0+Y*(A1+Y*(A2+Y*(A3+Y*A4))))*YTL
      Q(3)=BQ3+B2
      Q(4)=BQ4+B2
      SALL(2)=P(3)
      SALG(3)=P(4)
      I=3
       DX=GG
      H1=H**2
      H2=H1/12.0
      T(3)=P(3)*(1.0-H2*Q(3))
      T(4)=P(4)*(1.0-H2*Q(4))
      L(4)=T(4)-T(3)
      NCOUNT=3
      MINF=2
  440 I=I+1
C     IF END OF MESH IS REACHED, MODIFY TRIAL EIGENVALUE
      IF(I-MESH) 460,450,450
  450 IF(NDCR-NCROSS) 800,900,900
C     RETURN TO BEGINNING OF OUTWARD INTEGRATION IF NECESSARY
  460 Q(5) =GG(I)
      IF(IK-I)  700,700,500
```

```
  500 D(5)=D(4)+H1*Q(4)*P(4)
      T(5)=D(5)+T(4)
      IF(1.0-ABS(H2*Q(5))) 450,450,540
  540 P(5)=T(5)/(1.0-H2*Q(5))
      SALC(I) = P(5)
       IF(SIGN) 550,545,560
  545 NSTOP=545
      GO TO 9900
  550 IF(P(5)) 580,580,570
  560 IF(P(5)) 570,580,580
  570 NCROSS=NCROSS+1
C     COUNT CHANGES IN SIGN
      SIGN=-SIGN
  580 NCOUNT=NCOUNT+1
      IF(7-NCOUNT) 585,590,600
  585 NSTOP=585
      GO TO 9900
  590 NCOUNT=2
  600 NINT=NINT+1
      IF(40-NINT) 605,610,620
  605 NSTOP=605
      GO TO 9900
  610 DX=DX+DX
      H=DX
      H1=H**2
      H2=H1/12.0
      NINT=0
      T(5)=P(5)*(1.0-H2*Q(5))
      T(3)=P(3)*(1.0-H2*Q(3))
      D(5)=T(5)-T(3)
  620 DO 650 K=1,4
      P(K)=P(K+1)
      T(K)=T(K+1)
      D(K)=D(K+1)
  650 Q(K)=Q(K+1)
      GO TO 440
  700 IF(NCOUNT-2) 705,710,500
  705 NSTOP=705
      GO TO 9900
  710 IF(NINT-4) 500,500,720
C     MATCHING RADIUS HAS BEEN REACHED GOING OUT
C     IF NDCR NOT EQUAL TO NCROSS,MODIFY TRIAL EIGENVALUE
  720 EIGEN=E
      IF(NDCR-NCROSS) 800,1000,900
  800 MORE=1
C     TOO MANY CROSSINGS, INCREASE ABSF(E)
      MOREV=MOREV+1
      IF(MOREV-1) 805,830,820
```

```
  805 NSTOP=805
      GO TO 9900
  820 IF(E -EMORE) 830,840,840
  830 EMORE=E
  840  IF (LESS) 845,860,990
  845 NSTOP=845
      GO TO 9900
  860 E=1.25*EG
      GO TO 200
  900 LESS=1
C     TOO FEW CROSSINGS, DECREASE ABSF(E)
      LESSV=LESSV+1
       IF(LESSV-1) 905,920,910
  905 NSTOP=905
      GO TO 9900
  910 IF(ELESS- E) 920,930,930
  920 ELESS=E
  930 IF(MORE) 935,950,990
  935 NSTOP=935
      GO TO 9900
  950 E=0.75*EG
      GO TO 200
  990 E=0.5*(EMORE+ELESS)
      GO TO 200
 1000 IF(ABS(SNLO(I-1))-ABS(SNLO(I-2))) 1010,1040,1040
C     CHECK TO SEE THAT WAVE IS IN THE DAMPED REGION (ABSOLUTE VALUE
C     DECREASING AND SIGNS ALIKE)
 1010 IF (P(5)) 1020,500,1030
 1020 IF(SNLO(I-2)) 1100,500,500
 1030 IF(SNLO(I-2)) 500,500,1100
 1040 IF(1.0E+25 -ABS(P(5))) 900,900,500
C     LARGE ABSOLUTE VALUE OF P IN WHAT SHOULD BE THE DAMPED REGION
C       INDICATES TOO FEW PEAKS, DECREASE ABSF(E)
C     NOW NDCR = NCROSS AND MATCHING RADIUS LIES IN DAMPED REGION
 1100 IMATCH=I-2
      XMATCH=R(I-2)
      PPOUT=(T(4)-T(2)-0.5*(P(4)-P(2)))/H
      SZ=PPOUT/P(3)
C     INTEGRATION IS BY 8 APPLICATIONS OF NEWTON-COTES CLOSED
C       QUADRATURE FOR FIVE INTERVALS ON EACH BLOCK
C       XIFC =(5*H(BLOCK 1)/288)/2 ,H(1) =0.0025*SCALE FACTOR
      SUM1=0.0
      XIF=XIFC
      I=1
      VALUE=0.0
 1110 MM=8
      SUM2=0.0
      XIF=XIF+XIF
```

```
 1120 Y=VALUE
      VALUE=SNLO(I+5)**2
      SUM2=SUM2+19.0*(VALUE+Y)+75.0*(SNLO(I+4)**2+SNLO(I+1)**2)
     1  +50.0*(SNLO(I+2)**2+SNLO(I+3)**2)
      I=I+5
      IF(IMATCH-I) 1125,1150,1130
 1125 NSTOP=1125
      GO TO 9900
 1130 MM=MM-1
      IF(MM)1135,1140,1120
 1135 NSTOP=1135
      GO TO 9900
 1140 SUM1=SUM2*XIF+SUM1
      GO TO 1110
 1150 SUM1= SUM1+SUM2*XIF
 1160 SI=SUM1/P(3)**2
      PMATCH=P(3)
      IF(NN-1) 1165,1170,1180
 1165 NSTOP=1165
      GO TO 9900
 1170 XINW=EPL*XMATCH
C     FOR N =1, START INWARD INTEGRATION AT(8+LAM)*XMATCH OR X MAX
      GO TO 1200
 1180 XINW=FPL*XMATCH
C     FOR N NOT=1, START AT (5+LAM)*XMATCH OR X MAX (END OF MESH
 1200 DO 1220 I= 41,MESH,40
      IF(XINW-R(I)) 1210,1210,1220
 1210 KKK =I
      GO TO 1250
 1220 KKK =MESH
 1250 I =KKK
      DX =R(I-1)-R(I)
      H =DX
      XIF=0.17361111E-1*DX
      HSQ=H*H
      HSQ12=HSQ/12.0
      Q(3)= QQ(I)
      P(3)=EXP(-R(I)*SQRT(Q(3)))
 1260 SUM3=P(3)/Q(3)
      I=I-1
      Q(4) =QQ(I)
 1270 P(4)=EXP(-R(I)*SQRT(Q(4)))
      IF(ABS(P(4))-1.0E-35) 1280,1280,1300
 1280 KKK=KKK -40
      IF(KKK -IMATCH) 1290,1290,1250
 1290 WRITE(6,9030) Z ,NN,LAM,KKK
      P(3) = 1.0E-35
      KKK =KKK +40
```

```
      P(4 ) = 1.5E-35
1300  IF(PMATCH) 1310,1305,1320
1305  NSTOP=1305
      GO TO 9900
1310  P(3)=-P(3)
      P(4)=-P(4)
1320  SNLO(I+1)=P(3)
      SNLO(I)=P(4)
      T(3)=P(3)*(1.0-HSQ12 *Q(3))
      T(4)=P(4)*(1.0-HSQ12*Q(4))
      D(4)=T(4)-T(3)
1330  DO 1350 M=2,40
      I=I-1
      Q(5) =QQ(I)
      D(5) =HSQ*Q(4)*P(4)+D(4)
      T(5)=D(5)+T(4)
      P(5)=T(5)/(1.0-HSQ12*Q(5))
      IF(I-IMATCH+1) 1335,1400,1340
1335  NSTOP=1335
      GO TO 9900
1340  SNLO(I)=P(5)
      DO 1350 K=1,4
      P(K)=P(K+1)
      T(K)=T(K+1)
      D(K)=D(K+1)
1350  Q(K)=Q(K+1)
      Q(5) =QQ(I-2)
      D(5)=HSQ*Q(4)*P(4)+D(4)
      T(5)=D(5)+T(4)
       P(5)=T(5)/(1.0-HSQ12*Q(5))
     P(5)=1.09375*P(4)+0.2734375*P(5)-0.546875*P(3)+0.21875*P(2)-
    1  0.0390625*P(1)
      I=I-1
      DX=DX/2.0
      Q(5) =QQ(I)
      H=DX
      HSQ=H*H
      HSQ12=HSQ/12.0
      T(5)=P(5)*(1.0-HSQ12*Q(5))
      T(4)=P(4)*(1.0-HSQ12*Q(4))
      D(5)=T(5)-T(4)
      SNLO(I)=P(5)
      DO 1380 L=1,4
      P(L)=P(L+1)
      T(L)=T(L+1)
      D(L)=D(L+1)
1380  Q(L)=Q(L+1)
      GO TO 1330
```

```
C       MATCHING RADIUS HAS BEEN REACHED COMING IN
 1400 K=KKK
      VALUE=SNLC(K)*SNLC(K)
      GO TO 1420
 1410 SUM3=SUM3+XIF*SUM4
      XIF =XIF*0.5
 1420 MM=8
      SUM4 =0.0
 1430 Y=VALUE
      VALUE=SNLO(K-5)*SNLO(K-5)
      SUM4=SUM4+19.0*(VALUE+Y)+75.0*(SNLO(K-1)**2+SNLO(K-4)**2)
     1  +50.0*(SNLO(K-2)**2+SNLO(K-3)**2)
      K=K-5
       IF(K-IMATCH) 1435,1450,1440
 1435 NSTOP=1435
      GO TO 9900
 1440 MM=MM-1
      IF(MM) 1445,1410,1430
 1445 NSTOP=1445
      GO TO 9900
 1450 SUM3=SUM3+XIF*SUM4
      S3=SUM3/P(4)**2
      PPIN=(T(5)-T(3)-0.5*(P(5)-P(3)))/H
      S4=PPIN/P(4)
      DE=(S2-S4)/(S1-S3)
      DEPPP=DE/E
      IF(ABS(DE/E)-THRESH) 2000,1460,1460
 1460 E=E+DE
      IF(E) 200,1480,1480
 1480 E=E-DE
      WRITE(6,9670) E,DE
 9670 FORMAT(2F10.5)
      DE=0.50*DE
      GO TO 1460
C       IMPROVE TRIAL EIGENVALUE BY PERTURBATION THEORY IF NECESSARY
C       CALCULATE THE NORMALIZED WAVE FUNCTIONS
 2000 PCP=PMATCH/P(4)
      DO 2010 J=IMATCH,KKK
 2010 SNLC(J)=SNLC(J)*PCP
      SUM1=0.0
      J=1
      XIF=XIFC
      VALUE=0.0
 2020 MM=8
      XIF=XIF+XIF
      SUM2=0.0
 2030 Y=VALUE
      VALUE=SNLC(J+5)*SNLC(J+5)
```

```
      SUM2=SUM2+19.0*(VALUE+Y)+75.0*(SNLO(J+4)**2+SNLO(J+1)**2)
     1  +50.0*(SNLO(J+2)**2+SNLO(J+3)**2)
      J=J+5
      MM=MM-1
      IF(MM) 2035,2040,2030
 2035 NSTOP=2035
      GO TO 9900
 2040 SUM1=SUM1+XIF*SUM2
      IF(KKK-J) 2045,2050,2020
 2045 NSTOP=2045
      GO TO 9900
 2050 C1=SQRT(SUM1)
      IF(SNLO(3)) 2060,2055,2070
 2055 NSTOP=2055
      GO TO 9900
 2060 C1=-C1
 2070 DO 2080 I=1,KKK
 2080 SNLO(I)=SNLO(I)/C1
      RETURN
 9900 WRITE( 6,9020) NSTOP
      STOP
 9920 WRITE (6,9010) NN,LAM ,Z
      STOP
 9010 FORMAT (20H   NO CONVERGENCE ON,I4,I1,F4.0)
 9020 FORMAT(5HCSTOP,I4,8HIN SCHEQ)
 9030 FORMAT  (6HOAT Z=,F6.0,6H  NL =,I3,I1,7H  KKK =,I5,22H IS LESS THA
     1N IMATCH =,I5,43H INWARD INTEGRATION WILL BE TRIED AT KKK+40)
 9600 FORMAT(I4,2F12.5)
      END


      SUBROUTINE CROSYM(M)
C     SIMULTANEOUS EQUATION SOLVER
C     WRITTEN BY J.C. HANSON,SCIENTIFIC COMPUTATION DEPARTMENT,
C     LOCKHEED MISSLES AND SPACE COMPANY, SUNNYVALE, CALIFORNIA
C     SOLVE M SIMULTANEOUS EQUATIONS BY THE METHOD OF CROUT
      COMMON/COM1/V(521),R(521),RU(521),RU2(521),RU3(521),X(521),
     2  XI(521),XJ(521),RSCORE(521),RSATOM(521),RSVALE(521),
     3  RUINL1(521),RUINL2(521),RUFNL1(521),RUFNL2(521),RUEXCH(521),
     4  XNUM(521),DENM(521),SNLO(521),GG(521),RR(521),
     5  NNLZ(24),WWNL(24),NKKK(24),EE(24),A(4,5),SNL(24,521)
      N=M+1
      I1=1
  100 I3=I1
      SUM=ABS(A(I1,I1))
      DO 120 I=I1,M
      IF(SUM-ABS(A(I,I1))) 110,120,120
  110 I3=I
```

```
      SUM=ABS(A(I,I1))
  120 CONTINUE
      IF(I3-I1) 130,150,130
  130 DO 140 J=1,N
      SUM=-A(I1,J)
      A(I1,J)=A(I3,J)
  140 A(I3,J)=SUM
  150 I3=I1+1
      DO 160 I=I3,M
  160 A(I,I1)=A(I,I1)/A(I1,I1)
  170 J2=I1-1
      I3=I1+1
      IF(J2) 180,200,180
  180 DO 190 J=I3,N
      DO 190 I=1,J2
  190 A(I1,J)=A(I1,J)-A(I1,I)*A(I,J)
      IF(I1-M) 200,220,200
  200 J2=I1
      I1=I1+1
      DO 210 I=I1,M
      DO 210 J=1,J2
  210 A(I,I1)=A(I,I1)-A(I,J)*A(J,I1)
      IF(I1-M) 100,170,100
  220 DO 240 I=1,M
      J2=M-I
      I3=J2+1
      A(I3,N)=A(I3,N)/A(I3,I3)
      IF(J2) 230,250,230
  230 DO 240 J=1,J2
  240 A(J,N)=A(J,N)-A(I3,N)*A(J,I3)
  250 RETURN
      END
//GO.SYSIN DD *
```

```
// EXEC FCRTCLGF,REGION.GO=150K
//FORT.SYSIN DD *
C         POTENTIAL FROM THE SEPT 1969 FORM OF THE REPULSIVE POTENTIAL PROGRAM
C         HETERONUCLEAR FORM
      DIMENSION X(441),RL(441),XX(41),LL(41)                                MOD1
      DIMENSION R(1000),RR(1000),VP(1000),FPR2D(1000),APSI(1000)
      DIMENSION IH(20),C(2),BPSI(1000)
      COMMON/COM1/TX(40,11),TRU(40,11),DX(11),DR(11)                        MOD1
      COMMON/COM2/ AQ(1000),ADQ(1000),ARFO(1000),ARFT(1000),ARFOT(1000)     MOD1
      COMMON/COM3/ D,DD,DDR,DRS,FRR,DZ,RTEST,RT2,RS,HDRS,FDD,ZMAX           MOD9
      COMMON/COM4/ BQ(1000),BDQ(1000),BRHO(1000),BRFT(1000),BRFOT(1000)     MOD1
      CALL EP
      DO 1 I=1,1000
      R(I)=0.0
      RR(I)=0.0                                                             MOD6
      AQ(I)=0.0
      BQ(I)=0.0
      VP(I)=0.0
      ADQ(I)=0.0
      BDQ(I)=0.0
      ARFO(I)=0.0
      BRFO(I)=0.0
      ARFT(I)=0.0
      BRFT(I)=0.0
      ARFOT(I)=0.0
      BRFOT(I)=0.0
    1 FPR2D(I)=0.0
      PI=3.141593                                                             29 542
      TP=2.0*PI                                                               29 543
      TPR=1.0/TP                                                              29 544
      FT=5.0/3.0                                                              29 545
      FOT=4.0/3.0                                                             29 546
      SCD=2.871                                                               29 548
      SCX=0.7386                                                              29 549
      R3=1.0/3.0                                                              29 550
      R6=1.0/6.0                                                              29 551
      DX(1)=0.0025                                                            29 552
    2 READ(5,9010,END=9999) INUC,KSTEP,AZ,AI,BZ,BI,DM,RM,RTEST,DD,          MOD1
     X      FRR,FRS,IPN                                                      MOD1
 9010 FORMAT(I2,I3,2(F3.0,F2.0),3F2.0,3F5.1,I4)                             MOD9
      IF(INUC.LE.0) GO TO 9999
      TAZ=2.0*AZ                                                            MOD9
      TBZ=2.0*BZ                                                            MOD9
      DSS=0.0
      FKS=KSTEP                                                               29 569
      FKSR=1.0/FKS                                                            29 563
      DDK=FKS*DD                                                              29 570
      KSM=KSTEP-1                                                             29 564
```

```
      READ(5,9030) IH                                                    29 565
 9030 FORMAT(20A4)                                                       29 566
      DOUT=DM                                                           MOD9
      RS=DD                                                              29 557
      RT2=RTEST*RTEST                                                    29 558
      HDRS=0.5*DRS                                                       29 559
      ZMAX=RTEST                                                        MOD9
      DZ=DD                                                              29 561
      HDD=0.5*DD
      FPD=4.0*PI*DD                                                      29 567
      DDR=1.0/DD
      KM=DM*DDR
      KMM=KM-1
      RKM=1.0/KM                                                        MOD9
      KMR=KM*DDR                                                        MOD9
      KMRM=KMR-1
      RKMR=1.0/KMR
      VCOE=AZ*BZ                                                         29 814
      DVCOE=VCOE*RKMR
      CA=0.8853414/AZ**R3                                                29 572
      CB=0.8853414/BZ**R3                                                29 573
      C(1)=CA                                                            29 574
      C(2)=CB                                                            29 575
      N=1
      GO TO (5,5,5,4,390,396),INUC
    4 N=2
    5 DR(1)=DX(1)*C(N)
      DO 7 I=1,10
      DX(I+1)=DX(I)+DX(I)                                                29 579
    7 DR(I+1)=DR(I)+DR(I)
      IP2=1                                                              29 581
      IP3=1                                                              29 582
      IP4=1                                                              29 583
      IP5=1                                                              29 584
      IP6=1                                                              29 585
      IP7=1                                                              29 586
      IP8=1                                                              29 587
      IP9=1
      IP10=1                                                             29 589
      IP11=1                                                             29 590
      X(1)=0.0                                                           29 591
      RU(1)=0.0                                                          29 592
      K=1                                                                29 593
      DO 15 I=1,11                                                       29 594
      D=DX(I)                                                            29 595
      DO 10 J=1,40                                                       29 596
      K=K+1                                                              29 597
      X(K)=X(K-1)+D                                                      29 598
```

```
   10 CONTINUE                                                          29 599
   15 CONTINUE                                                          29 600
      READ(5,9020) (RU(I),I=1,441)                                      29 601
 9020 FORMAT(5E15.7)                                                    29 603
      WRITE(6,9500)                                                     29 607
 9500 FORMAT(1H1)                                                       29 604
      WRITE(6,9510) (RU(I),I=1,441)                                     29 602
 9510 FORMAT(10F10.5)                                                   29 605
 9520 FORMAT(5X,10F10.5)                                                29 606
      M=1                                                               29 608
      DO 19 J=1,11                                                      29 609
      DO 18 I=1,40                                                      29 610
      TX(I,J)=X(M)*C(N)                                                 29 611
      TRU(I,J)=RU(M)                                                    29 612
   18 M=M+1                                                             29 613
   19 CONTINUE                                                          29 614
      GO TO 150                                                         29 615
   20 GO TO (21,22,23),IP2                                              29 616
   21 IP2=2                                                             29 617
      CALL FILL(1,1)                                                    29 618
      GO TO 200                                                         29 619
   22 IP2=3                                                             29 620
      CALL FILL(1,21)                                                   29 621
      GO TO 200                                                         29 622
   23 IP2=1                                                             29 623
      GO TO (31,32,33),IP3                                              29 624
   31 IP3=2                                                             29 625
      CALL FILL(2,1)                                                    29 626
      GO TO 21                                                          29 627
   32 IP3=3                                                             29 628
      CALL FILL(2,21)                                                   29 629
      GO TO 21                                                          29 630
   33 IP3=1                                                             29 631
      GO TO (41,42,43),IP4                                              29 632
   41 IP4=2                                                             29 633
      CALL FILL(3,1)                                                    29 634
      GO TO 31                                                          29 635
   42 IP4=3                                                             29 636
      CALL FILL(3,21)                                                   29 637
      GO TO 31                                                          29 638
   43 IP4=1                                                             29 639
      GO TO (51,52,53),IP5                                              29 640
   51 IP5=2                                                             29 641
      CALL FILL(4,1)                                                    29 642
      GO TO 41                                                          29 643
   52 IP5=3                                                             29 644
      CALL FILL(4,21)                                                   29 645
      GO TO 41                                                          29 646
```

```
   53 IP5=1                                                              29 647
      GO TO (61,62,63),IP6                                               29 648
   61 IP6=2                                                              29 649
      CALL FILL(5,1)                                                     29 650
      GO TO 51                                                           29 651
   62 IP6=3                                                              29 652
      CALL FILL(5,21)                                                    29 653
      GO TO 51                                                           29 654
   63 IP6=1                                                              29 655
      GO TO (71,72,73),IP7                                               29 656
   71 IP7=2                                                              29 657
      CALL FILL(6,1)                                                     29 658
      GO TO 61                                                           29 659
   72 IP7=3                                                              29 660
      CALL FILL(6,21)                                                    29 661
      GO TO 61                                                           29 662
   73 IP7=1                                                              29 663
      GO TO (81,82,83),IP8                                               29 664
   81 IP8=2                                                              29 665
      CALL FILL(7,1)                                                     29 666
      GO TO 71                                                           29 667
   82 IP8=3                                                              29 668
      CALL FILL(7,21)                                                    29 669
      GO TO 71                                                           29 670
   83 IP8=1                                                              29 671
      GO TO (91,92,93),IP9                                               29 672
   91 IP9=2                                                              29 673
      CALL FILL(8,1)                                                     29 674
      GO TO 81                                                           29 675
   92 IP9=3                                                              29 676
      CALL FILL(8,21)                                                    29 677
      GO TO 81                                                           29 678
   93 IP9=1                                                              29 679
      GO TO (101,102,103),IP10                                           29 680
  101 IP10=2                                                             29 681
      CALL FILL(9,1)                                                     29 682
      GO TO 91                                                           29 683
  102 IP10=3                                                             29 684
      CALL FILL(9,21)                                                    29 685
      GO TO 91                                                           29 686
  103 IP10=1                                                             29 687
      GO TO (111,112,113),IP11                                           29 688
  111 IP11=2                                                             29 689
      CALL FILL(10,1)                                                    29 690
      GO TO 101                                                          29 691
  112 IP11=3                                                             29 692
      CALL FILL(10,21)                                                   29 693
      GO TO 101                                                          29 694
```

```
113 IF11=1                                                              29 695
    GO TO 300                                                           29 696
150 CONTINUE                                                            29 697
    RDX=1.0/DX(1)                                                       29 698
    RT=0.0                                                              29 700
    K=0                                                                 29 701
    NFS=0                                                               29 704
    J=41                                                                29 705
    UU(41)=0.0                                                          29 706
    XX(41)=1.0E10                                                       29 707
160 RT=RT+DD                                                            29 708
    K=K+1                                                               29 709
    IF(KMR.LT.K) GO TO 300                                             MOD9
170 IF(J-41) 230,180,9999                                               29 711
180 IF(K-1) 9999,200,20                                                 29 712
200 XX(1)=XX(41)                                                        29 713
    UU(1)=UU(41)                                                        29 714
    DO 210 I=2,41                                                       29 715
    XX(I)=TX(I-1,1)                                                     29 716
210 UU(I)=TRU(I-1,1)                                                    29 717
    J=1                                                                 29 718
220 J=J+1                                                               29 719
    IF(J-41) 230,230,20                                                 29 720
230 IF(RT-XX(J)) 250,240,220                                            29 721
240 R(K)=RT                                                             29 722
    RR(K)=1.0/RT                                                       MOD6
    FPR2D(K)=FPD*RT*RT                                                  29 723
    IF(N-1) 9999,245,345                                                29 724
245 ADQ(K)=DD*UU(J)                                                     29 725
    GO TO 260                                                           29 726
250 R(K)=RT                                                             29 727
    RR(K)=1.0/RT                                                       MOD6
    FPR2D(K)=FPD*RT*RT                                                  29 728
    IF(N-1) 9999,255,355                                                29 729
255 ADQ(K)=DD*((RT-XX(J-1))*RDX*(UU(J)-UU(J-1))+UU(J-1))                29 730
260 ARHO(K)=ADQ(K)/FPR2D(K)                                             29 731
    APSI(K)=SQRT(ARHO(K))                                               29 732
    ARFT(K)=ARHO(K)**FT                                                 29 733
    ARFCT(K)=ARHO(K)**FCT                                               29 734
    J=J-1                                                               29 735
    IF(K-1) 9999,270,280                                                29 736
270 AQ(K)=ADQ(K)                                                        29 737
    GO TO 160                                                           29 738
280 AQ(K)=AQ(K-1)+ADQ(K)                                                29 739
    GO TO 160                                                           29 740
300 CONTINUE                                                            29 741
    IF(N-1) 9999,310,320                                                29 742
310 WRITE(6,9550)  AZ,AI
```

```
 9550 FORMAT(1H1,20X,'NUCLEAR CHARGE WAS',F4.0,', THE ATOM WAS',F4.0,' T
     2IMES IONIZED',//)
      WRITE(6,9580) ((R(I),ADQ(I),AQ(I),ARHO(I)),I=1,KMR)
 9580 FORMAT(3(F8.3,2F10.5,E10.2))                                      29 747
      WRITE(6,9500)
      GO TO (390,4,400,400), INUC
  320 WRITE(6,9555)  BZ,BI
 9555 FORMAT(1HO,20X,'NUCLEAR CHARGE WAS',F4.0,', THE ATOM WAS',F4.0,' T
     2IMES IONIZED',//)
      WRITE(6,9580) ((R(I),BDQ(I),BQ(I),BRHO(I)),I=1,KMR)
      WRITE(6,9500)
      GO TO 400
  345 BDQ(K)=DD*UU(J)                                                   29 749
      GO TO 360                                                         29 750
  355 BDQ(K)=DD*((RT-XX(J-1))*RDX*(UU(J)-UU(J-1))+UU(J-1))              29 751
  360 BRHO(K)=BDQ(K)/FPR2D(K)                                           29 752
      BPSI(K)=SQRT(BRHO(K))                                             29 753
      BRFT(K)=BRHO(K)**FT                                               29 754
      BRFOT(K)=BRHO(K)**FOT                                             29 755
      J=J-1                                                             29 756
      IF(K-1) 9999,370,380                                              29 757
  370 BQ(K)=BDQ(K)                                                      29 758
      GO TO 160                                                         29 759
  380 BQ(K)=BQ(K-1)+BDQ(K)                                              29 760
      GO TO 160                                                         29 761
  390 DO 395 I=1,KM                                                     29 762
      BQ(I)=AQ(I)                                                       29 763
      BDQ(I)=ADQ(I)                                                     29 764
      BRHO(I)=ARHO(I)                                                   29 765
      BPSI(I)=APSI(I)                                                   29 766
      BRFT(I)=ARFT(I)                                                   29 767
  395 BRFOT(I)=ARFOT(I)                                                 29 768
      GO TO 400
  396 DO 399 K=1,KM
      AQ(K)=BQ(K)
      ADQ(K)=BDQ(K)
      ARHO(K)=BRHO(K)
      APSI(K)=BPSI(K)
      ARFT(K)=BRFT(K)
  399 ARFOT(K)=BRFOT(K)
  400 CONTINUE                                                          29 770
  410 WRITE(6,9530) IH
 9530 FORMAT(1H1,20X,20A4,//,30X,'HETERONUCLEAR MODEL, AUGUST 1969 FORM'
     X  ,//)
  500 CONTINUE                                                          29 773
      WRITE (6,9540) DZ,DRS,FRR,RTEST,DD,KSTEP,RM                       MOD9
 9540  FORMAT(10X,'DZ=',F6.3,',DRS=',F6.3,',FRR=',F5.2,',RTEST WAS',
     2  F5.2,', DD WAS',F6.3,', RUN EVERY',I3,' STEPS, RMAX =',F5.2,//) MOD9
```

```
      D=DSS                                                                  29 788
      WRITE(6,9650)
 9650 FORMAT('       D       VP          VSZ         EDD         EXX         VC
     2     VSNC       VNN         VNE         VEE         UA          USNA'/)
      DO 1000 K=KSTEP,KM,KSTEP                                               29 791
      D=D+DDK                                                                29 792
      RD=1.0/D                                                              MOD9
      TCD=2.0*RD                                                            MOD9
      HRD=0.5*RD                                                            MOD9
      HD2=0.5*D*D                                                           MOD9
      VNN=VCCE*TCD                                                          MOD9
      DVNN=DVCCE*TOD                                                        MOD9
      VSZ=0.0                                                               MOD9
      VNE=0.0
      VEE=0.0
      DO 600 I=1,KMRM
      DVSZ=DVNN                                                             MOD9
      JI=I-K                                                                MOD9
      JP=I+K                                                                MOD9
      IF(JP.LE.KMRM) GO TO 510
      JP=KMRM
  510 JPP=JP+1                                                              MOD9
      IF(JI) 545,540,535                                                    MOD9
  535 VCA=BQ(JI)*RR(I)                                                      MOD9
      VCB=AQ(JI)*RR(I)                                                      MOD9
      DVNE=-(TAZ*BDQ(I)+TBZ*ADQ(I))*RR(I)
      GO TO 550                                                             MOD9
  540 JI=1                                                                  MOD9
      VCA=0.0                                                               MOD9
      VCB=0.0                                                               MOD9
      DVNE=-(TAZ*BDQ(I)+TBZ*ADQ(I))*RR(I)
      GO TO 550                                                             MOD9
  545 JI=-JI                                                                MOD9
      VCA=BQ(JI)*RD                                                         MOD9
      VCB=AQ(JI)*RD                                                         MOD9
      DVNE=-(TAZ*BDQ(I)+TBZ*ADQ(I))*RD                                      MOD9
  550 DVSZ=DVSZ+DVNE
      VNE=VNE+DVNE
      CC1=D-0.5*R(I)-HD2*RR(I)
      CC2=1.0+D*RR(I)                                                       MOD9
      CC3=-0.5*RR(I)                                                        MOD9
      VBA1=0.0                                                              MOD9
      VBA2=0.0                                                              MOD9
      VBA3=0.0                                                              MOD9
      VBB1=0.0                                                              MOD9
      VBB2=0.0                                                              MOD9
      VBB3=0.0                                                              MOD9
      DO 560 J=JI,JP                                                        MOD9
```

```
      VBA1=VBA1+BDQ(J)*RR(J)                                          MOD9
      VBB1=VBB1+ADQ(J)*RR(J)                                          MOD9
      VBA2=VBA2+BDQ(J)                                                MOD9
      VBB2=VBB2+ADQ(J)                                                MOD9
      VBA3=VBA3+BDQ(J)*R(J)                                           MOD9
  560 VBB3=VBB3+ADQ(J)*R(J)                                           MOD9
      VEA=HRD*(CC1*VBA1+CC2*VBA2+CC3*VBA3)                            MOD9
      VEB=HRD*(CC1*VBB1+CC2*VBB2+CC3*VBB3)
      VAB=0.0
      VAA=0.0                                                         MOD9
      DO 570 J=JPP,KMR
      VAA=VAA+BDQ(J)*RR(J)                                            MOD9
  570 VAB=VAB+ADQ(J)*RR(J)                                            MOD9
      DVEE=ADQ(I)*(VAA+VBA+VCA)+BDQ(I)*(VAB+VBB+VCB)
      VEE=VEE+DVEE
  600 VSZ=VSZ+DVEE+DVSZ
      VSZ=VSZ+DVNN
      VSNC=VNN+VEE+VNE
      VSNA=VNN+0.5*VNE                                                MOD7
      CALL CLAP(EDD,EXX,FT,FOT,KMR)
      VDXC=2.0*(EDD-EXX)                                              MOD9
      VSN=VSNC+VDXC
      VP(K)=VSZ+VDXC
      VDXA=R3*(EDD-2.0*EXX)
      VA=VSNA+VDXA                                                    MOD1
      WRITE(6,9600) D,VP(K),VSZ,EDD,EXX,VSN,VSNC,VNN,VNE,VEE,VA,VSNA
 9600 FORMAT(F10.3,11F10.3)                                           MOD6
      IF(K-KSTEP) 9999,620,700                                        MOD6
  620 DIS=0.0                                                         MOD6
      VSNCD=VSZ*D                                                     MOD9
      DO 650 I=1,KSM
      DIS=DIS+DD
  650 VP(I)=VSNCD/DIS+VDXC
      GO TO 1000
  700 KL=K-KSTEP
      DVP=(VP(KL)-VP(K))*FKSR
      DO 750 I=1,KSM
  750 VP(KL+I)=VP(KL+I-1)-DVP
 1000 CONTINUE                                                                29 825
      IF(IPN) 1010,2,1010
 1010 CONTINUE
      WRITE(7,9610) (IH(I),I=1,15),KM
 9610 FORMAT(' DIFFERENT,TRUE ',15A4,I4)
      WRITE(7,9630) (APSI(I),I=1,20)                                  MOD7
 9630 FORMAT(10F8.4)                                                  MOD7
      WRITE(7,9635) (APSI(I),I=21,KM)                                 MOD7
 9635 FORMAT(10F8.5)                                                  MOD7
      WRITE(7,9630) (BPSI(I),I=1,20)                                  MOD7
```

```
      WRITE(7,9635) (BPSI(I),I=21,KM)                                    MOD7
      WRITE(7,9660) (IH(I),I=1,15),KM                                    MOD7
 9660 FORMAT(' POTENTIAL FROM ',15A4,I4)                                 MOD7
      WRITE(7,9640) (VP(I),I=1,20)                                       MOD7
 9640 FORMAT(5F12.4)                                                     MOD7
      WRITE(7,9645) (VP(I),I=21,KM)                                      MOD7
 9645 FORMAT(8F10.5)                                                     MOD7
      GO TO 2
 9999 STOP                                                                29 837
      END                                                                 29 838


      SUBROUTINE FILL(N,M)
      COMMON/COM1/TX(40,11),TRU(40,11),DX(11),DR(11)                      29 840
      NN=N+1                                                              29 841
      JJ=0                                                                29 842
      DO 100 I=1,37,2                                                     29 843
      MM=M+JJ                                                             29 844
      MP=MM+1                                                             29 845
      TRU(I,N)=TRU(MM,NN)                                                 29 846
      TX(I,N)=TX(MM,NN)                                                   29 847
      IP=I+1                                                              29 848
      TX(IP,N)=TX(I,N)+DR(N)                                              29 849
      TRU(IP,N)=0.5*(TRU(I,N)+TRU(MP,NN))                                 29 850
  100 JJ=JJ+1                                                             29 851
      MP=M+19                                                             29 852
      MPP=M+20                                                            29 853
      TRU(39,N)=TRU(MP,NN)                                                29 854
      TX(39,N)=TX(MP,NN)                                                  29 855
      TX(40,N)=TX(39,N)+DR(N)                                             29 856
      TRU(40,N)=2.0*TRU(39,N)-TRU(38,N)                                   29 857
      RETURN                                                              29 858
      END                                                                 29 962


      SUBROUTINE OLAP(EDD,EXX,FT,FOT,KMR)
      COMMON/COM2/ AQ(1000),ADQ(1000),ARHO(1000),ARFT(1000),ARFOT(1000)  MOD1
      COMMON/COM3/ D,DD,DDR,DRS,FRR,DZ,RTEST,RT2,RS,HDRS,HDD,ZMAX        MOD9
      COMMON/COM4/ BQ(1000),BDQ(1000),BRHO(1000),BRFT(1000),BRFOT(1000)  MOD1
       EDD=0.0                                                           MOD9
      EXX=0.0                                                            MOD9
      Z=D-RTEST
      R=RS
      DR=DRS
  100 R2=R*R                                                             MOD9
      RA=R2+Z*Z                                                          MOD9
      IF(RA.GT.RT2) GO TO 200                                            MOD9
      RE=R2+(D-Z)**2                                                     MOD9
```

```
      IF(RB.GT.RT2) GO TO 200                                          MOD9
      RA=SQRT(RA)
      RB=SQRT(RB)
      I=RA*DDR+HDD
      J=RB*DDR+HDD
      RDR=R*DR
      DR=DR*FRR
      IF(I.LT.1) I=1
      IF(J.LT.1) J=1
      IF(I.GT.KMR) GO TO 200
      IF(J.GT.KMR) GO TO 200
      EDD=EDD+((ARHO(I)+BRHO(J))**FT-ARFT(I)-BRFT(J))*RDR
      EXX=EXX+((ARHO(I)+BRHO(J))**FOT-ARFOT(I)-BRFOT(J))*RDR           MOD9
  150 R=R+DR
      GO TO 100
  200  Z=Z+DZ
      IF(Z.GT.ZMAX) GO TO 1000                                         MOD9
      IF(ABS(Z)-DD) 260,250,220                                        MOD9
  220 IF(ABS(Z-D).GE.DD) GO TO 260                                     MOD9
  250 R=RS
      DR=DRS
      GO TO 100
  260 R=DD
      DR=HDRS
      GO TO 100
 1000 EDD=18.03902*DZ*EDD                                              MOD9
      IF(EDD.LT.0.0) EDD=0.0                                           MOD9
      EXX=4.64076*DZ*EXX                                               MOD9
      IF(EXX.LT.0.0) EXX=0.0                                           MOD9
      RETURN                                                           MOD9
      END
//GO.FTC6F001 DD SYSOUT=A,DCB=BLKSIZE=133
//GO.SYSIN DD *
```

```
// EXEC FCRTCLGP,REGION.GO=100K
//FORT.SYSIN DD *
C
C       THIS PROGRAM COMPUTES THE DISTRIBUTION OF IMPACT PARAMETERS
C
        FX(R,THETA)=R*COS(THETA-PHI)-(YR*SIN(PHI)+XR*COS(PHI))
        FY(R,THETA)=R*SIN(THETA-PHI)+(XR*SIN(PHI)-YR*COS(PHI))
        DIMENSION IA1(1500 ),A5(4,4),A6(6,3),B1(3),B2(3),B3(6),
       1K1(6),IS(6),S(6)
        DIMENSION LARGE(6)
        INTEGER TAU,ALFA,RN1
        LOGICAL*1 CHAR(80)
1       READ(5,557,END=999) CHAR
        READ(5,900) ICODE,A,B,INUMBR
        READ(5,955) LARGE
        READ(5,901) SCALEF,RNA,RCL
        DO 2 I=1,3
2       READ(5,901) (A5(I,J),J=1,2)
        DO 3 I=1,INUMBR
3       READ(5,902) (A6(I,J),J=1,3)
        READ(5,903) PHI,XR,YR,ALPHA,RMAX
        WRITE(6,900) ICODE,A,B,INUMBR
        WRITE(6,901) SCALEF,RNA,RCL
        DO 990 I=1,3
990     WRITE(6,901) (A5(I,J),J=1,2)
        DO 991 I=1,INUMBR
991     WRITE(6,902) (A6(I,J),J=1,3)
        WRITE(6,903) PHI,XR,YR,ALPHA,RMAX
900     FORMAT(I3,2F10.4,I3)
901     FORMAT(3F10.4)
902     FORMAT(3F10.4)
903     FORMAT(5F10.4)
955     FORMAT(6I2)
950     FORMAT(' ZERO CHECK 1')
557     FORMAT(80A1)
C
        ALFA=2**16+3
        RN1=2*(2**30-2)+1
        NN=1
        TAU=1
        SCALE2=RNA/RCL
C       THIS SECTION GIVES GRID ON WHICH TC WORK
C
        IA=A/.005
        IB=B/.005
C
C       THIS STATEMENT INTIALIZES IA1(I) TC ZERO
C
```

```
      PFR=.005/SCALEF
      PFR1=SCALEF/.005
      DO 5 I=1,1500
5     IA1(I)=0
C
C     THIS SECTION CONVERTS ATOM POSITIONS TO SCALED COORDINATES
C
      DO 10 I=1,INUMBR
      DO 9 J=1,3
9     A6(I,J)=A6(I,J)*PFR1
      WRITE(6,950)
10    CONTINUE
      IF (ICODE-2)  51,20,999
C
C     THIS SECTION CONVERTS VERTICES INTO SCALED COORDINATES
C
20    DO 25 I=1,3
      DO 24 J=1,2
24    A5(I,J)=A5(I,J)*PFR1
25    CONTINUE
C
C      CRITX IS THE X VALUE AT WHICH WE CHANGE THE CONDITIONS WHICH MUST BE
C     MET IF THE GRIDED COORDINATE IS TO FALL IN THE REPRESENTATIVE AREA.
C
      CRITX=A5(2,1)
C
C     THIS SECTION CALCULATES THE EQUATIONS OF THE LINES BOUNDING THE TRIANGLE
C
      DO 35 I=1,2
      B1(I)=(A5(I+1,2)-A5(I,2))/(A5(I+1,1)-A5(I,1))
      WRITE(6,950)
35    B2(I)=(A5(I,2)-B1(I)*A5(I,1)+A5(I+1,2)-B1(I)*A5(I+1,1))/2.0
      B1(3)=0.0
      B2(3)=A5(3,2)
C
C     THIS SECTION CALCULATES THE NEW COORDINATES OF THE ATOMS IN THE
C     REPRESENTATIVE AREA
C
51    DO 50 I=1,INUMBR
      IF (A6(I,1)) 40,44,40
40    THETA=ATAN(A6(I,2)/A6(I,1))
      WRITE(6,950)
      GO TO 45
44    THETA=1.5707963
45    R=SQRT(A6(I,2)**2+A6(I,1)**2)
      A6(I,1)=FX(R,THETA)
50    A6(I,2)=FY(R,THETA)*COS(ALPHA)-A6(I,3)*SIN(ALPHA)
      WRITE(6,650) ((A6(I,J),J=1,3),I=1,INUMBR)
```

```
650   FORMAT(3F10.3)
C
C     THIS SECTION CALCULATES THE ACTUAL DISTRIBUTION OF IMPACT PARAMETERS
C
      IX=IA+1
      IXX=IB+1
      DO 75 I=1,IX
      DO 74 J=1,IXX
      ACK1=I-1
      ACK2=J-1
      IF (ICODE-2) 54,53,54
53    IF (ACK2-CRITX) 100,100,150
100   IF (ACK1-(B1(1)*ACK2+B2(1)))54,54,74
150   IF (ACK1-(B1(2)*ACK2+B2(2))) 54,54,74
54    IF (ACK2) 55,60,55
55    THETA = ATAN(ACK1/ACK2)
      GO TO 65
60    THETA=1.707963
65    R=SQRT(ACK1**2+ACK2**2)
      ACK1=FY(R,THETA)*COS(ALPHA)
      ACK2=FX(R,THETA)
C
C     THIS SECTION CALCULATES THE SHORTEST IMPACT PARAMETER AND
C     ASSIGNS IT TO THE CORRECT ATOM
C
      RANGE=6.25E04
      KEEP=0
      DO 180 K=1,INUMBR
      B3(K)=(A6(K,1)-ACK2)**2+(A6(K,2)-ACK1)**2
      IF(LARGE(K)-1) 179,178,999
178   B3(K)=B3(K)*SCALE2
179   IF(B3(K)-RANGE) 182,192,180
182   RANGE=B3(K)
      KEEP=K
      GO TO 180
192   CALL RANDOM(0.0,2.0,2.0,5.0,TAU,2.0,0,NN,ALFA,RN1,SN,SN1)
      IF (.5-SN) 180,555,555
555   RANGE=B3(K)
      KEEP=K
180   CONTINUE
      IF (LARGE(KEEP)-1) 186,185,999
185   RANGE=RANGE/SCALE2
186   IRANGE= SQRT(RANGE)+1.0
      ITALLY= (KEEP-1)*250+IRANGE
      IA1(ITALLY)=IA1(ITALLY)+1
74    CONTINUE
75    CONTINUE
      DO 360 I=1,INUMBR
```

```
      ISUM=0
      IS(I)=0
      JMIN=(I-1)*250+1
      JMAX=JMIN+249
      DO 299 J=JMIN,JMAX
299   ISUM=ISUM+IA1(J)
      IS(I)=ISUM
360   CONTINUE
      WRITE(6,556) CHAR
556   FORMAT('1',23X,80A1,///)
      WRITE(7,550) CHAR
550   FORMAT(80A1)
      DO 347 I=1,INUMBR
      JMIN=(I-1)*250+1
      J1=JMIN+19
      J2=J1+20
      J3=J2+20
      J4=J3+20
      J5=J4+20
      J6=J5+20
      J7=J6+20
      J8=J7+20
      J9=J8+20
      J0=J9+20
      JJ1=J0+20
      JJ2=JJ1+20
      JJ3=JJ2+10
      WRITE(6,951)(IA1(J),J=JMIN,J1)
      WRITE(7,951)(IA1(J),J=JMIN,J1)
      JMIN=J1+1
      WRITE(6,951)(IA1(J),J=JMIN,J2)
      WRITE(7,951)(IA1(J),J=JMIN,J2)
      JMIN=J2+1
      WRITE(6,951)(IA1(J),J=JMIN,J3)
      WRITE(7,951)(IA1(J),J=JMIN,J3)
      JMIN=J3+1
      WRITE(6,951)(IA1(J),J=JMIN,J4)
      WRITE(7,951)(IA1(J),J=JMIN,J4)
      JMIN=J4+1
      WRITE(6,951)(IA1(J),J=JMIN,J5)
      WRITE(7,951)(IA1(J),J=JMIN,J5)
      JMIN=J5+1
      WRITE(6,951)(IA1(J),J=JMIN,J6)
      WRITE(7,951)(IA1(J),J=JMIN,J6)
      JMIN=J6+1
      WRITE(6,951)(IA1(J),J=JMIN,J7)
      WRITE(7,951)(IA1(J),J=JMIN,J7)
      JMIN=J7+1
```

```
      WRITE(6,951)(IA1(J),J=JMIN,J8)
      WRITE(7,951)(IA1(J),J=JMIN,J8)
      JMIN=J8+1
      WRITE(6,951)(IA1(J),J=JMIN,J9)
      WRITE(7,951)(IA1(J),J=JMIN,J9)
      JMIN=J9+1
      WRITE(6,951)(IA1(J),J=JMIN,J0)
      WRITE(7,951)(IA1(J),J=JMIN,J0)
      JMIN=J0+1
      WRITE(6,951)(IA1(J),J=JMIN,JJ1)
      WRITE(7,951)(IA1(J),J=JMIN,JJ1)
      JMIN=JJ1+1
      WRITE(6,951)(IA1(J),J=JMIN,JJ2)
      WRITE(7,951)(IA1(J),J=JMIN,JJ2)
      JMIN=JJ2+1
      WRITE(6,951)(IA1(J),J=JMIN,JJ3)
      WRITE(7,951)(IA1(J),J=JMIN,JJ3)
951   FORMAT(2014)
      WRITE(7,914)
914   FORMAT(' NEW ATOM')
      WRITE(6,915)
915   FORMAT('0',20X,'TOTAL NUMBER OF IMPACT POINTS TALLIED',///)
      WRITE(6,913) I,IS(I)
913   FORMAT(28X,'ATOM',I1,'=',I5,' POINTS',///)
347   WRITE(6,558)
558   FORMAT('1')
      GO TO 1
999   STOP
      END


      SUBROUTINE RANDOM(A,B,SIGMA,MU,TAU,LAMBDA,G,NN,ALFA,
     1          RN1,SN,SN1)
C
C     SUBROUTINE RANDOM GENERATES THREE PSEUDORANDOM NUMBER DISTRIBU-
C     TIONS: 1) UNIFORM, 2) NORMAL, 3) EXPONENTIAL.  IF TAU=1,2,3,
C     ONE GETS A UNIFORM,NORMAL , EXPONENTIAL DIST. RESP.  A DEFFINITION
C     OF THE OTHER TERMS USED IN THIS ROUTINE MAY BE FOUND IN THESIS
C     BOOK 1, K.L. ALLEN.  THE ROUTINE WAS TAKEN FROM RALSTON AND WILF
C     NUMERICAL METHODS FOR DIGITAL COMPUTERS.
C
      INTEGER TAU,ALFA,G,RN,RN1
      REAL MU,LAMBDA
1     RN=RN1*ALFA
      RSTN=RN
      RSTN=RSTN*2.0**(-31)
      IF (TAU-2) 2,3,4
C     EXPONENTIAL DISTRIBUTION
```

```
2       IF(RSTN) 9,9,8
9       RSTN=ABS(RSTN)
8       SN=-(1.0/LAMBDA)*ALOG(RSTN)
        SN=ABS(SN)
        GO TO 5
C       UNIFORM DISTRIBUTION
3       SN=(B-A)*RSTN+A
        SN=ABS(SN)
        GO TO 5
C       NORMAL DISTRIBUTION
4       IF (G-1) 7,6,7
7       NN=NN+1
        G=G+1
        RN1=RN
        RSTN1=RSTN
        GO TO 1
6       IF (RSTN1) 11,11,10
11      RSTN1=ABS(RSTN1)
10      Z=SQRT(-2.0*ALOG(RSTN1))*SIGMA
        SN1=Z*COS(6.28318*RSTN)+MU
        SN=Z*SIN(6.28318*RSTN)+MU
        G=0
5       NN=NN+1
        RN1=RN
        RETURN
        END
//GO.SYSIN DD *
```

```
// EXEC FORTCLGP,REGION.GO=150K
//FORT.SYSIN DD *
C
C       THIS PROGRAM TAKES THE RAW DATA FROM THE IMPACT PARAMETER PROGRAM
C       AND GENERATES A LEAST SQUARES POLYNOMIAL FIT THROUGH THE POINTS.
C       SPECIFICALLY, THE PROGRAM SELECTS THE POINT AT WHICH THE
C       DISTRIBUTION IS A MAXIMUM AND FITS A STRAIGHT LINE THROUGH ALL
C       POINTS PRECEDING THIS POINT AND A TENTH DEGREE POLYNOMIAL TO ALL
C       POINTS FOLLOWING THIS POINT.  THE FIT IS ACCOMPLISHED BY
C       GENERATING THE ORTHOGONAL POLYNOMIALS (LEGENDRE) ASSOCIATED WITH
C       THE FUNCTION.
C
C       DATA INPUT: CARD 1; NUMBER OF POINTS TO BE FITTED, ID NUMBER
C       INDICATING IF CARD AND GRAPHICAL OUTPUT IS WANTED (1=NO,2=YES);
C       CARD2,3: TWO CARDS WITH INFORMATION TO BE OUTPUTED WITH GRAPH...
C       MUST BE INSERTED FOR EVERY RUN;CARD4-N: DATA FROM THE DISTRIBUTION
C       OF IMPACT PARAMETER PROGRAM
C
        COMMON/POLY/NTERMS,B(300),C(300),D(300)
        DIMENSION X(300),F(300),W(300),ERROR(300),PJM1(300),PJ(300)
        DIMENSION XX(300),YY(300),YY1(300),XX1(300),IIF(300)
        DIMENSION IIF1(300)
        REAL LAST
        REAL*8 TITLE(12)
        REAL LABEL/'F(X)'/
        REAL LABEL1/'P(X)'/
        REAL LABEL2/'E(X)'/
1       READ(5,899,END=999) NPOINT,IFLAG
899     FORMAT(2I4)
        READ(5,950) TITLE
950     FORMAT(6A8)
        READ(5,900) (IIF(I),I=1,NPOINT)
900     FORMAT(20I4)
        WRITE(6,907)
907     FORMAT('1')
        NTERMS=2
        ICOUNT=0
        NFT=NPOINT
        KEEP=0
C
C       NTERMS=DEGREE OF FIT+1; ICOUNT= A COUNTER;KEEP= VALUE AT WHICH
C       THE IMPACT PARAMETER DISTRIBUTION IS A MAXIMUM; IRANGE= THE RANGE
C       CORRESPONDING TO THE MAXIMUM IMPACT PARAMETER;
C
        IRANGE=0
        DO 777 I=1,NPOINT
        IF (IRANGE-IIF(I)) 778,778,777
778     KEEP=I
```

```
      IRANGE=IIF(I)
777   CONTINUE
      WRITE(6,9000) KEEP
9000  FORMAT(' ',25X,'KEEP= ',I5,///)
      NPOINT=KEEP
101   ICOUNT=ICOUNT+1
      IF (ICOUNT.EQ.2) GO TO 779
780   GO TO 102
779   DO 787 I=1,NPOINT
787   IIF1(I)=PJ(I)
      NTERMS=11
      NPOINT=NPT-NPOINT
      DO 781 I=1,NPOINT
781   IIF(I)=IIF(KEEP+I)
C
C     X(I)= X VALUES OF DISTRIBUTION TO BE FITTED; F(I)= VALUES OF THE
C     FUNCTION CORRESPONDING TO X;W(I)= WEIGHTING FACTORS FOR THE
C     ORTHOGONAL POLYNOMIALS;
C
102   DO 5 I=1,NPOINT
      ACK=I
      X(I)=ACK*.005
      F(I)=IIF(I)
      W(I)=1.0
5     CONTINUE
      CALL ORTPOL(NPOINT,X,F,W,ERROR,PJM1,PJ)
      WRITE(6,601)(J,B(J),C(J),D(J),J=1,NTERMS)
601   FORMAT(' ',25X,I4,3D16.8)
      DO 60 I=1,NPOINT
      IIF(I)=F(I)
60    PJ(I)=ORTVAL(X(I))
      WRITE(6,600) (X(I),IIF(I),PJ(I),ERROR(I),I=1,NPOINT)
600   FORMAT(' ',10X,F5.3,I4,F10.5,E13.3,//)
      IF (IFLAG.EQ.1) GO TO 72
      IF (IFLAG.EQ.2) GO TO 73
73    CALL DRAW(NPOINT ,X,F,1,0,LABEL,TITLE,.1, 40.0,1,0,2,2,8,12,0,
     1   LAST)
      CALL DRAW(NPOINT ,X,PJ,2,0,LABEL1,TITLE,.1, 40.0,1,0,2,2,8,12,0,
     1  LAST)
      CALL DRAW(NPOINT ,X,ERROR,3,0,LABEL2,TITLE,.1, 40.0,1,0,2,2,8,12,
     1   0,LAST)
72    IF (ICOUNT.EQ.2) GO TO 888
      GO TO 101
888   DO 889 I=1,NPOINT
889   IIF1(I+KEEP)=PJ(I)
74    WRITE(7,900) (IIF1(I),I=1,NPT)
      GO TO 1
999   STOP
```

```
      END

      FUNCTION ORTVAL(X)
C
C     SUBROUTINE ORTVAL EVALUATES THE ORTHOGONAL POLYNOMIALS AT A
C     SPECIFIED VALUE OF X
C
      COMMON/POLY/NTERMS,B(300),C(300),D(300)
      K=NTERMS
      ORTVAL=D(K)
      PREV=0.
10    K=K-1
      IF (K.EQ.0)     RETURN
      PREV2=PREV
      PREV=ORTVAL
      ORTVAL=D(K)+(X-B(K))*PREV-C(K+1)*PREV2
      GO TO 10
      END


      SUBROUTINE ORTPOL(NPOINT,X,F,W,ERROR,PJM1,PJ)
C
C     SUBROUTINE ORTPOL CALCULATES THE COEFFICIENTS OF THE TERMS IN
C     THE ORTHOGONAL POLYNOMIAL USED IN THE LEAST SQUARES FIT
C
      COMMON/POLY/NTERMS,B(300),C(300),D(300)
      DIMENSION X(300),F(300),W(300),ERROR(300),PJM1(300),PJ(300)
      DIMENSION S(300)
C
      DO 9 J=1,NTERMS
      B(J)=0.
      D(J)=0.
9     S(J)=0.
      C(1)=0.
      DO 10 I=1,NPOINT
      D(1)=D(1)+F(I)*W(I)
      B(1)=B(1)+X(I)*W(I)
10    S(1)=S(1)+W(I)
      D(1)=D(1)/S(1)
      DO 11 I=1,NPOINT
11    ERROR(I)=F(I)-D(1)
      IF (NTERMS.EQ.1)     RETURN
      B(1)=B(1)/S(1)
      DO 12 I=1,NPOINT
      PJM1(I)=1.
12    PJ(I)=X(I)-B(1)
      J=1
```

```
C
20      J=J+1
        DO 21 I=1,NPOINT
        P=PJ(I)*W(I)
        D(J)=D(J)+ERROR(I)*P
        P=P*PJ(I)
        B(J)=B(J)+X(I)*P
21      S(J)=S(J)+P
        D(J)=D(J)/S(J)
        DO 22 I=1,NPOINT
22      ERROR(I)=ERROR(I)-D(J)*PJ(I)
        IF (J.EQ. NTERMS)       RETURN
        B(J)=B(J)/S(J)
        C(J)=S(J)/S(J-1)
        DO 27 I=1,NPOINT
        P=PJ(I)
        PJ(I)=(X(I)-B(J))*PJ(I)-C(J)*PJM1(I)
27      PJM1(I)=P
        GO TO 20
        END
//GO.FT06F001 DD SYSOUT=A,SPACE=(CYL,(3,1))
//GO.SYSIN DD *
```

```
// EXEC FORTCLG,REGION.GO=150K
//FORT.SYSIN DD *
C       PROGRAM INLOSS
        DIMENSION BMAX(3),PUD(3),ARO(3),LM(3),TFL(3),XM(3),KXM(3)          7JOB,722
        DIMENSION FLP(750),FLPD(750,3),BCNI(20,20),BCZZ(400)               7JOB,723
        DIMENSION IH1(20),IH2(4),IAH(4),PSE(8),FIT(8),EAV(3)               7JOB,724
        DIMENSION EA(20),ENN(20),EN(20),BC(40),LCLT(40),IH3(19),IH4(19)    7JOB,725
        DIMENSION E(100),ERN(100),DREL(100),PP(100),EL(100),ET(100)        7JOB,726
        DIMENSION RHO(1000),EIN(1000),ELEC(1000),FN(1000),RX(1000),        7JOB,727
       2          RX2(1000),RX2R(1000),RMIN(1000),B(1000)                 7JOB,728
        DIMENSION V(1000),SIG(1000),APSI(1000),BPSI(1000)                  7JOB,729
        DIMENSION ELECS(30,3),PEL(30,3),ECLT(30)                           7JOB,730
        EQUIVALENCE(BCNI,BCZZ)                                             7JOB,731
        START=0.01*ITIME(XX)
        CALL EP
        DO 1 I=1,100
        E(I)=0.0
        ERN(I)=0.0
        EL(I)=0.0
        ET(I)=0.0
        EA(I)=0.0
        LCLT(I)=0.0
      1 DREL(I)=0.0
        DO 2 I=1,1000
        RHO(I)=0.0
        EIN(I)=0.0
        ELEC(I)=0.0
        FN(I)=0.0
        RX(I)=0.0
        RX2(I)=0.0
        RX2R(I)=0.
        RMIN(I)=0.
        B(I)=0.0
        V(I)=0.0
        SIG(I)=0.0
        APSI(I)=0.
      2 BPSI(I)=0.
        HBAR=1.05443E-27                                                   7JOB,733
        PI=3.14159265                                                      7JOB,734
        ECHRG=4.80286E-10                                                  7JOB,735
        CVD=0.529172E-8                                                    7JOB,736
        CVE=1.6021E-12                                                     7JOB,737
        CVM=1.67239E-24                                                    7JOB,738
        CAH=1.0E-8/CVD                                                     7JOB,739
        ECT=8.0/3.0                                                        7JOB,740
        FCT=4.0/3.0                                                        7JOB,741
        KSTEP=5
 9000 FORMAT(A4,I2,9F6.4,3I3,I4,F7.4)
```

```
      READ (5,9000) LCRYST,LTPE,(BMAX(I),I=1,3),(PUD(I),I=1,3),          7JOB,742
     2  (ARO(I),I=1,3),(LM(I),I=1,3),KM,FACL                            7JOB,743
      PUDM=AMAX1(PUD(1),PUD(2),PUD(3))
      PUDM2=PUDM*PUDM                                                    7JOB,745
      DO 5 I=1,3                                                         7JOB,746
      LF=LM(I)                                                           7JOB,747
 9010 FORMAT(20F4.0)                                                     7JOB,748
      READ (5,9010) (FLP(L),L=1,LF)                                      7JOB,749
      PT=0.0                                                             7JOB,750
      DO 3 L=1,LF                                                        7JOB,751
    3 PT=PT+FLP(L)                                                       7JOB,752
      TFL(I)=PT                                                          7JOB,753
      SF=ARO(I)/PT                                                       7JOB,754
      DO 5 L=1,LF                                                        7JOB,755
      FLPD(L,I)=FLP(L)*SF                                                7JOB,756
    5 CONTINUE                                                           7JOB,757
      BMM=AMAX1(BMAX(1),BMAX(2),BMAX(3))
      READ (5,9020) IH1                                                  7JOB,760
 9020 FORMAT(20A4)                                                       7JOB,761
      READ(5,9025) IH3,KMR                                               7JOB,762
 9025 FORMAT(19A4,I4)                                                    7JOB,763
      READ(5,9030) (APSI(I),I=1,KMR)                                     7JOB,764
 9030 FORMAT(10F8.5)                                                     7JOB,765
      READ(5,9030) (BPSI(I),I=1,KMR)                                     7JOB,766
      READ(5,9025) IH4,KMV                                               7JOB,767
      READ(5,9032) (V(I),I=1,20)                                         7JOB,768
 9032 FORMAT(5F12.5)                                                     7JOB,769
      READ(5,9035) (V(I),I=21,KMV)                                       7JOB,770
 9035 FORMAT(8F10.5)                                                     7JOB,771
      KMVR=MINO(KM,KMV,KMR)                                              7JOB,772
      KMVRP=KMVR+1                                                       7JOB,773
      KMVP=KMV+1                                                         7JOB,774
      KMM=KM-1                                                           7JOB,775
      KMP=KM+1                                                           7JOB,776
      FKMP=KMP                                                           7JOB,777
      KMD=KM+KM                                                          7JOB,778
      DX=0.02
      TDX=3.0*DX                                                         7JOB,780
      DX2=DX*DX                                                          7JOB,781
      DXR=1.0/DX                                                         7JOB,782
      FK=KMVP                                                            7JOB,784
      XMV=FK*DX                                                          7JOB,785
      HDX=0.5*DX                                                         7JOB,786
      DBS=0.005                                                          7JOB,787
      DBSR=1.0/DBS                                                       7JOB,788
 9040 FORMAT(10F8.4)                                                     7JOB,789
      READ (5,9050) (EA(N),N=11,18),IAH                                  7JOB,790
 9060 FORMAT(I10)                                                        7JOB,791
```

```
      READ(5,9040) (EA(N),N=1,10)                                          7JCB,792
 9050 FORMAT(8F8.4,4A4)                                                    7JCB,793
      READ (5,9060) JFIT                                                   7JCB,794
      IF(JFIT) 9999,15,10                                                  7JCB,795
 9070 FORMAT(16F5.3)                                                       7JCB,796
   10 READ(5,9070) (PSE(J),FIT(J),J=1,JFIT)                               7JCB,797
 9080 FORMAT(2F4.0,2F8.4,2F3.0,I4,F7.3,2I3,2F3.0,F5.0,6X,4A4)              7JCB,798
   15 READ(5,9080) ZB,ZT,BMAS,TMAS,EOS,DEC,KEOM,AC,LSKIP,NM,RES,DRE,REM,7JCB,799
    2  IH2                                                                7JCB,800
      IF(ZB) 9999,9999,20                                                  7JCB,801
   20 ACA=AO/0.529172                                                      7JCB,802
      HACA=0.5*ACA                                                         7JCB,803
      IIFIT=3                                                              7JCB,804
      RCA=FACL*ACA                                                         7JCB,805
      RCDB=RCA/DBS                                                         7JCB,806
      AM=TMAS/BMAS                                                         7JCB,807
      BM=BMAS*CVM/CVE                                                      7JCB,808
      COM=AM/(1.0+AM)                                                      7JCB,809
C                       ERY=1000.0/13.605                                  7JCB,810
      ERY=73.5023888                                                       7JCB,811
      CEC=COM*ERY                                                          7JCB,812
C                     7.28926 = .75*PI*(3*PI**2)**1/3                      7JCB,813
      ECCC=1.0
      EIC=ECCC*7.28926*DX*HBAR/(CVE*CVC)
      TCBM=2.0/BM                                                          7JCB,815
      EC=EOS                                                               7JCB,816
      ECEV=EOS*1000.                                                       7JCB,817
      DECEV=DEC*1000.                                                      7JCB,818
      FL=LSKIP                                                             7JCB,819
      DBL=0.01*FL                                                          7JCB,820
      DBR=1.0/DBL                                                          7JCB,821
      BML=BMM*RCA                                                          7JCB,822
      LML=BML*DBSR                                                         7JCB,823
      SCB=DBL*DBSR                                                         7JCB,824
      KLB=PUDM*DXR*RCA
      L2SKIP=LSKIP+LSKIP                                                   7JCB,825
      L3SKIP=L2SKIP+LSKIP                                                  7JCB,826
      L4SKIP=L3SKIP+LSKIP                                                  7JCB,827
      NE=0                                                                 7JCB,828
      DO 25 I=1,3                                                          7JCB,829
      XM(I)=RCA*SQRT(BMAX(I)**2+PUD(I)**2)                                 7JCB,830
   25 KXM(I)=XM(I)*DXR+HDX                                                 7JCB,831
      KLM=MAXO(KXM(1),KXM(2),KXM(3))                                       7JCB,832
      KLM=MINO(KLM,KM)                                                     7JCB,833
      KLMM=KLM-1                                                           7JCB,834
C                   MAKE THE RUSSEK ENERGY-ELECTRON PRODUCTION TABLE       7JCB,835
      DO 30 M=1,40                                                         7JCB,836
      BC(M)=0.0                                                            7JCB,837
```

```
   30 LCLT(M)=0.0                                                    7JCB,838
      NMP=NM+1                                                       7JCB,839
      NMM=NM-1                                                       7JCB,840
      WRITE(6,9505) IH2                                              7JCB,841
 9505 FORMAT(1H1,52X,4A4,//)                                         7JCB,842
      BC(1)=NM                                                       7JCB,843
      ENN(1)=EA(1)                                                   7JCB,844
      EN(1)=EA(1)                                                    7JCB,845
      DO 40 N=2,NM                                                   7JCB,846
      IF(EA(N)-1.0E-10) 42,42,37                                     7JCB,847
   37 ENN(N)=ENN(N-1)+EA(1)*EA(N)                                    7JCB,848
      FFN=N
      EN(N)=ENN(N)/FFN
      J=NMP-N                                                        7JCB,851
      FJ=J                                                           7JCB,852
      J=N-1                                                          7JCB,853
   40 BC(N)=FJ*BC(J)/FFN
      GO TO 45                                                       7JCB,855
   42 NM=N-1                                                         7JCB,856
      NMP=NM+1                                                       7JCB,857
      NMM=NM-1                                                       7JCB,858
   45 WRITE (6,9510) IH1,IAH,LCRYST,AO,KM,DX                         7JCB,859
 9510 FORMAT(27X,20A4,/,20X,4A4,' IONIZATION ENERGIES, ',A4,' LATTICE.
     2 LATTICE CONSTANT WAS ',F6.3,/,36X,' DONE WITH ',I4,' STEPS, AND',
     3 F6.3,' BOHR STEP SIZE',/)
      DO 47 M=1,400                                                  7JCB,865
   47 BCZZ(M)=0.0                                                    7JCB,866
      DRER=1.0/DRE                                                   7JCB,863
      FDE=(REM-RES)*DRER+1.001
      JM=FDE                                                         7JCB,867
      JMM=JM-1                                                       7JCB,868
      E(1)=RES                                                       7JCB,869
      ERN(1)=(1.0/E(1))**NMM                                         7JCB,870
      DO 50 J=2,JM                                                   7JCB,871
      E(J)=E(J-1)+DRE                                                7JCB,872
   50 ERN(J)=(1.0/E(J))**NMM                                         7JCB,873
      DO 200 N=1,NM                                                  7JCB,874
      NR=NM-N                                                        7JCB,875
      BCNI(N,1)=-NR                                                  7JCB,876
      NRP=NR+1                                                       7JCB,877
      IF(NR-2) 200,200,60                                            7JCB,878
   60 DO 100 I=2,NR                                                  7JCB,879
      FI=I                                                           7JCB,880
      K=NRP-I                                                        7JCB,881
      FK=K                                                           7JCB,882
  100 BCNI(N,I)=-BCNI(N,I-1)*FK/FI                                   7JCB,883
  200 CONTINUE                                                       7JCB,884
      DO 500 L=1,JM                                                  7JCB,885
```

```
      DO 202 I=1,100                                                    7JCB,886
  202 PP(I)=0.0                                                         7JCB,887
      PZ=1.0                                                            7JCB,888
      PZT=0.0                                                           7JCB,889
      FK=E(L)/EN(1)                                                     7JCB,890
      K=FK                                                              7JCB,891
      IF(K-NM) 210,210,205                                              7JCB,892
  205 K=NM                                                              7JCB,893
  210 DO 220 I=1,K                                                      7JCB,894
      FI=I                                                              7JCB,895
  220 PZT=PZT+(-1.0**I)*((E(L)-FI*EN(1))**NMM)*BC(I)                    7JCB,896
      PZ=PZ+PZT*ERN(L)                                                  7JCB,897
      DO 400 N=1,NMM                                                    7JCB,898
      IF(LCUT(N)) 400,290,400
  290 IF(E(L)-ENN(N)) 400,390,300
  300 NP=N+1                                                            7JCB,900
      FK=(E(L)-ENN(N))/EN(NP)                                           7JCB,901
      K=FK                                                              7JCB,902
      IF(K) 390,390,310                                                 7JCB,903
  310 IF(K-NMM) 320,320,315                                             7JCB,904
  315 K=NMM                                                             7JCB,905
  320 DO 350 I=1,K                                                      7JCB,906
      FI=I                                                              7JCB,907
      EF=E(L)-ENN(N)-FI*EN(NP)                                          7JCB,908
      IF(EF) 390,350,350                                                7JCB,909
  350 PP(N)=PP(N)+(EF**NMM)*BCNI(N,I)                                   7JCB,910
  390 PP(N)=BC(N)*(((E(L)-ENN(N))**NMM)+PP(N))*ERN(L)                   7JCB,911
  400 CONTINUE                                                          7JCB,912
      IF(PZ) 410,420,420                                                7JCB,913
  410 PZ=0                                                              7JCB,914
  420 PPT=PZ                                                            7JCB,915
      DO 430 N=1,NM                                                     7JCB,916
      IF(PP(N)) 425,430,430                                             7JCB,917
  425 PP(N)=0.0                                                         7JCB,918
      LCUT(N)=-1
  430 PPT=PPT+PP(N)                                                     7JCB,919
      PPTR=1.0/PPT                                                      7JCB,920
      PZ=PPTR*PZ                                                        7JCB,921
      EL(L)=0                                                           7JCB,922
      ET(L)=0                                                           7JCB,923
      DO 440 N=1,NM                                                     7JCB,924
      PP(N)=PP(N)*PPTR                                                  7JCB,925
      FFN=N                                                             7JCB,926
      TE=PP(N)*FFN                                                      7JCB,927
      EL(L)=EL(L)+TE                                                    7JCB,928
  440 ET(L)=ET(L)+TE*EN(N)                                              7JCB,929
  450 CONTINUE                                                          7JCB,930
  500 CONTINUE                                                          7JCB,931
```

```
      DE1=E(1)-EA(1)                                                    7JCB,932
      DE1R=1.0/DE1                                                      7JCB,933
      FDEL=EL(1)*DE1R                                                   7JCB,934
      DO 650 J=1,JMM                                                    7JCB,935
  650 DREL(J)=DRER*(EL(J+1)-EL(J))                                      7JCB,936
C                   MAKE THE CROSS SECTION TABLE                        7JCB,937
      K=KMR                                                             7JCB,938
      KMH=KM/2                                                          7JCB,939
      KH=KMR-KMH                                                        7JCB,940
      FK=K                                                              7JCB,941
      XMP=DX*FKMP                                                       7JCB,942
      X=DX*FK                                                           7JCB,943
      XDX=X*DX
      SIG(KM)=0.0                                                       7JCB,945
      DO 700 M=1,KH                                                     7JCB,946
      K=K-1                                                             7JCB,947
      XDX=XDX-DX2                                                       7JCB,948
  700 SIG(KM)=SIG(KM)+XDX*(APSI(K)+BPSI(K))**EOT
      K=KM                                                              7JCB,950
      J=KMH                                                             7JCB,951
      KP=KMH-1                                                          7JCB,952
      DO 750 M=1,KP                                                     7JCB,953
      XDX=XDX-DX2                                                       7JCB,954
      J=J-1                                                             7JCB,955
      K=K-2                                                             7JCB,956
  750 SIG(K)=SIG(K+2)+XDX*(APSI(J)+BPSI(J))**EOT
      SIG(1)=SIG(2)+0.5*DX2*(APSI(1)+BPSI(1))**EOT
      DO 800 K=3,KMM,2                                                  7JCB,959
  800 SIG(K)=0.5*(SIG(K+1)+SIG(K-1))                                    7JCB,960
      WRITE(6,9820) (SIG(K),K=1,KMR)
      WRITE(6,9820) (V(K),K=1,KMV)
 9820 FORMAT(1X,10F11.5)
C                   MAKE CALCULATIONS FOR A SINGLE ION ENERGY
      WRITE(6,9505) IH2
 1000 DO 2900 NE=1,NEOM                                                 7JCB,962
      DO 1010 L=1,1000                                                  7JCB,963
      E(L)=0.0
      RMIN(L)=0.0
      EIN(L)=0.0                                                        7JCB,964
      ELEC(L)=0.0                                                       7JCB,965
 1010 CONTINUE                                                          7JCB,966
      DO 1020 M=1,3                                                     7JCB,967
 1020 EAV(M)=0.0                                                        7JCB,968
      VC=SQRT(ECEV*TOBM)                                                7JCB,969
      EIP=EIO*VC                                                        7JCB,970
      ECP=EO*CEC                                                        7JCB,971
      ECPR=1.0/ECP                                                      7JCB,972
C                   LOCATE THE DISTANCE OF CLOSEST APPROACH             7JCB,973
```

```
      K=KMVP                                                            7JCB,974
      X=XMV                                                             7JCB,975
      DO 1050 M=1,KMV                                                   7JCB,976
      K=K-1                                                             7JCB,977
      X=X-DX                                                            7JCB,978
      FN(K)=1.0-EOPR*V(K)                                               7JCB,979
      IF(FN(K)) 1060,1040,1040                                          7JCB,980
 1040 RX(K)=X                                                           7JCB,981
      RX2(K)=X*X                                                        7JCB,982
      RX2R(K)=1.0/RX2(K)                                                7JCB,983
 1050 CONTINUE                                                          7JCB,984
      X=DX                                                              7JCB,985
      KMIN=1                                                            7JCB,986
      GO TO 1065                                                        7JCB,987
 1060 KMIN=K                                                            7JCB,988
 1065 X=X+DX                                                            7JCB,989
      KMPO=KMIN+1                                                       7JCB,990
      DO 1070 M=1,KMIN                                                  7JCB,991
      RX(M)=0.0                                                         7JCB,992
      RX2(M)=0.0                                                        7JCB,993
      RX2R(M)=0.0                                                       7JCB,994
      FN(M)=0.0                                                         7JCB,995
 1070 CONTINUE                                                          7JCB,996
      RX(KMIN)=X-DX                                                     7JCB,997
      DXT=DX                                                            7JCB,998
      DO 1090 M=1,5                                                     7JCB,999
      DXT=0.1*DXT                                                       7JCB,000
      DO 1080 MM=1,10                                                   7JCB,001
      X=X-DXT                                                           7JCB,002
      POT=V(K)+(X-RX(K))*DXR*(V(K+1)-V(K))                              7JCB,003
      IF(1.0-EOPR*POT) 1090,1080,1080                                   7JCB,004
 1080 CONTINUE                                                          7JCB,005
 1090 X=X+DXT                                                           7JCB,006
      RMIN(1)=X                                                         7JCB,007
      B(1)=0.0                                                          7JCB,008
      KSS=KMIN-1                                                        7JCB,009
      PSI=0.0                                                           7JCB,010
C                THIS IS THE INTEGRAL WITH ZERO IMPACT PARAMETER        7JCB,011
      FSI=0.5*SQRT(FN(KMPO))*SIG(KMPO)                                  7JCB,012
      FIO=FSI*(RX(KMPO)-X)*DXR                                          7JCB,013
      DO 1100 K=KMPO,KLB                                                7JCB,014
      T=SIG(K)*SQRT(FN(K))                                              7JCB,015
 1100 PSI=PSI+T                                                         7JCB,016
      EIN(1)=EIF*(PSI+FSI-0.5*T+FIO)                                    7JCB,017
C          CALCULATE THE NUMBER OF ELECTRONS FROM THE RUSSEK MODEL       7JCB,018
      M=EIN(1)*DRER                                                     7JCB,019
      IF(M-1) 1110,1140,1140                                            7JCB,020
 1110 IF(EIN(1)-EA(1)) 1120,1120,1130                                   7JCB,021
```

```
 1120 ELEC(1)=0.0                                                    7JCB,022
      GO TO 1170                                                     7JCB,023
 1130 ELEC(1)=(EIN(1)-EA(1))*FDEL                                    7JCB,024
      GO TO 1150                                                     7JCB,025
 1140 ELEC(1)=EL(M)+(EIN(1)-E(M))*DREL(M)                            7JCB,026
 1150 DO 1160 I=1,3                                                  7JCB,027
 1160 EAV(I)=ELEC(1)*FLPD(1,I)                                       7JCB,028
 1170 EMAX=0.0                                                       7JCB,029
      LMAX=0                                                         7JCB,030
C                  THIS IS THE INTEGRAL FOR A SINGLE B(L)
      DO 1990 L=2,LML,LSKIP                                          7JCB,032
      LS=L                                                           7JCB,033
C                       FIND RC FOR GIVEN B(L)                      7JCB,034
      B(L)=B(L-LSKIP) +DBL                                           7JCB,035
      IF(B(L)-BML) 1171,1171,2000                                    7JCB,036
 1171 K=KSS+KSTEP
      X=RX(K)
      B2=B(L)*B(L)                                                   7JCB,039
      DO 1172 M=1,KSTEP
      K=K-1                                                          7JCB,041
      IF(1.0-ECPR*V(K)-B2*RX2R(K)) 1173,1173,1172                    7JCB,042
 1172 CONTINUE                                                       7JCB,043
 1173 KSS=K                                                          7JCB,044
      X=RX(K+1)                                                      7JCB,045
      DXT=DX                                                         7JCB,046
      DO 1175 M=1,3                                                  7JCB,047
      DXT=0.1*DXT                                                    7JCB,048
      DO 1174 MM=1,10                                                7JCB,049
      X=X-DXT                                                        7JCB,050
      POT=V(K)+(X-RX(K))*DXR*(V(K+1)-V(K))                           7JCB,051
      IF(1.0-ECPR*POT-B2/(X*X))  1175,1174,1174                      7JCB,052
 1174 CONTINUE                                                       7JCB,053
 1175 X=X+DXT                                                        7JCB,054
      RC=X                                                           7JCB,055
      RC2=RO*RO                                                      7JCB,056
C                       FIRST INCREMENT AT SINGULARITY FOR B(L)
      KT=ROA*DXR*SQRT(PUDM2+B2)                                      7JCB,058
      IF(KT-KLMM) 1177,1177,1176                                     7JCB,059
 1176 KT=KLMM                                                        7JCB,060
 1177 RMIN(L)=RC                                                     7JCB,061
      KB=K+2                                                         7JCB,062
      DRB=0.1*(RX(KB)-RO)                                            7JCB,063
 1180 DRBR=1.0/DRB                                                   7JCB,064
      DLC=0.5*RO*DX                                                  7JCB,065
      CB=2.0*RC2*DXR
      DL=0.5*SQRT(DX/RC)                                             7JCB,067
      POT=V(K)+(RO-RX(K))*DXR*(V(K+1)-V(K))                          7JCB,068
      SIGR=SIG(K)+(RO-RX(K))*DXR*(SIG(K+1)-SIG(K))                   7JCB,069
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```
      AL=1.0-ECPR*POT                                                   7JCB,070
      RN=RO+DRB                                                         7JCB,071
      POT=V(K)+(RN-RX(K))*DXR*(V(K+1)-V(K))                             7JCB,072
      AN=1.0-ECPR*POT                                                   7JCB,073
      M=C                                                               7JCB,074
      DADX=(AN-AL)*DRBR                                                 7JCB,075
      IF(DADX) 2000,2000,1182                                           7JCB,076
 1182 PSI=0.5*SIGR*AL*DU/SQRT(2.0*(DADX*RO2*RO+B2))                     7JCB,077
C                  INTEGRATE THE REST OF THE FIRST STEP FOR B(L)
      RN=RO                                                             7JCB,079
      DO 1190 M=1,10                                                    7JCB,080
      RN=RN+DRB                                                         7JCB,081
      AL=AN                                                             7JCB,082
      POT=V(K)+(RN-RX(K))*DXR*(V(K+1)-V(K))                             7JCB,083
      AN=1.0-ECPR*POT                                                   7JCB,084
      C=RO/RN                                                           7JCB,085
      U2=1.0-C                                                          7JCB,086
      U=SQRT(U2)                                                        7JCB,087
      DL=DUC/SQRT(RN*RN*RN*(RN-RO))                                     7JCB,088
      SIGR=SIG(K)+(RN-RX(K))*DXR*(SIG(K+1)-SIG(K))                      7JCB,089
 1185 T=SIGR*AN*DU/(C*C*SQRT(RO2*(AN-AL))/U2+B2*(2.0-U2))               7JCB,090
 1190 PSI=PSI+T                                                         7JCB,091
 1200 CONTINUE                                                          7JCB,092
      EIN(L)=EIF*CB*(PSI-0.5*T)                                         7JCB,093
      AN=FN(KB)                                                         7JCB,094
      PSI=0.5*SIG(KB)*AN/SQRT(AN-B2*RX2R(KB))                           7JCB,095
C                  COMPLETE THE INTEGRAL FOR B(L)                     7JCB,096
      KEP=KB+1                                                          7JCB,097
      DO 1290 K=KBP,KT                                                  7JCB,098
      T=SIG(K)*FN(K)/SQRT(FN(K)-B2*RX2R(K))                             7JCB,099
 1290 PSI=PSI+T                                                         7JCB,100
      EIN(L)=EIN(L)+EIF*(PSI-0.5*T)                                     7JCB,101
C            CALCULATE ELECTRONS FROM RUSSEK MODEL FOR THIS B(L)
      M=EIN(L)*DREB                                                     7JCB,103
      IF(M-1) 1410,1440,1440                                            7JCB,104
 1410 IF(EIN(L)-EA(1)) 1420,1420,1430                                   7JCB,105
 1420 ELEC(L)=0.0                                                       7JCB,106
      GO TO 1600                                                        7JCB,107
 1430 ELEC(L)=(EIN(L)-EA(1))*FDEL                                       7JCB,108
      GO TO 1500                                                        7JCB,109
 1440 IF(M-JM) 1460,1460,1450                                           7JCB,110
 1450 M=JM                                                              7JCB,111
 1460 ELEC(L)=(EIN(L)-E(M))*DREL(M)+EL(M)                               7JCB,112
C            ADD ELECTRONS FROM THIS B(L) TO AVERAGE
 1500 DO 1590 I=1,3                                                     7JCB,113
      IF(B(L)-BMAX(I)) 1510,1510,1590                                   7JCB,114
 1510 J=B(L)*DBSR                                                       7JCB,115
      EAV(I)=EAV(I)+ELEC(L)*FLPD(J,I)*SCB                               7JCB,116
```

```
1590 CONTINUE                                                          JOB,117
1600 IF(EIN(L)-EMAX) 1690,1690,1610                                    JOB,118
1610 EMAX=EIN(L)                                                       JOB,119
     LEMAX=L                                                           JOB,120
1690  CONTINUE                                                         JOB,121
9927 FORMAT(I20)
1990  CONTINUE                                                         JOB,122
     NOUT=0                                                            JOB,123
2000 WRITE(6,9540)                                                     JOB,124
     WRITE(6,9560) EOEV,(EAV(I),I=1,3)                                 JOB,125
     WRITE(6,9570)                                                     JOB,126
9570 FORMAT(2X,4('        B       RO  ENERGY  N(E)'))
     IF(LS-L4SKIP) 2040,2050,2050                                      JOB,128
2040 LS=L4SKIP                                                         JOB,129
2050 DO 2100 K=1,LS,L4SKIP                                             JOB,130
     L=K+LSKIP                                                         JOB,131
     M=K+L2SKIP                                                        JOB,132
     N=K+L3SKIP                                                        JOB,133
2100 WRITE (6,9550) B(K),RMIN(K),EIN(K),ELEC(K),B(L),RMIN(L),EIN(L),   JOB,134
    2 ELEC(L),B(M),RMIN(M),EIN(M),ELEC(M),B(N),RMIN(N),EIN(N),ELEC(N)  JOB,135
9550 FORMAT(2X,4(F9.3,F7.3,F7.1,F6.3))
     DO 2150 I=1,3                                                     JOB,137
2150 ELECS(NE,I)=EAV(I)                                                JOB,138
     ECUT(NE)=EOEV                                                     JOB,139
     ECEV=EOEV+DEOEV                                                   JOB,140
     EC=EO+DEO                                                         JOB,141
9500 FORMAT(1H1)                                                       JOB,143
     WRITE(6,9505) IH2                                                 JOB,145
2900 CONTINUE                                                          JOB,144
     WRITE (6,9510) IH1,IAH,LCRYST,AO,KM,DX                            JOB,146
     WRITE(6,9534) IH3                                                 JOB,147
     WRITE(6,9534) IH4                                                 JOB,148
9534 FORMAT(22X,19A4)                                                  JOB,149
     WRITE (6,9520) EA(1),NM                                           JOB,150
9520 FORMAT(40X,'THRESHOLD WAS ',F7.3,',',I5,' ELECTRONS WERE USED'//,
    2   10X,4('   E-TFF     N(E)      E(N) '))
     DO 2950 J=1,JM,4                                                  JOB,153
     JP1=J+1                                                           JOB,154
     JP2=J+2                                                           JOB,155
     JP3=J+3                                                           JOB,156
2950 WRITE(6,9530) E(J),EL(J),ET(J),E(JP1),EL(JP1),ET(JP1),            JOB,157
    2    E(JP2),EL(JP2),ET(JP2),E(JP3),EL(JP3),ET(JP3)                 JOB,158
9530 FORMAT(10X,4(F8.1,F9.4,F9.2))                                     JOB,159
     WRITE (6,9540)                                                    JOB,160
9540 FORMAT(/40X,'   ENERGY    N100(E)   N110(E)   N111(E)')
     WRITE (6,9560) (ECUT(I),(ELECS(I,J),J=1,3),I=1,KEOM)              JOB,162
9560 FORMAT(40X,F9.1,3F10.3)                                           JOB,163
3000 IF(JFIT) 15,15,3100                                               JOB,164
```

```
 3100 DO 3500 I=1,JFIT                                                  JOB,165
      FIX=FIT(I)/ELECS(KEOM,IIFIT)                                      JOB,166
      DO 3200 M=1,3                                                     JOB,167
      DO 3200 N=1,KEOM                                                  JOB,168
 3200 PEL(N,M)=FIX*ELECS(N,M)+PSE(I)                                    JOB,169
      WRITE(6,9505) IH2
      WRITE (6,9510) IH1,IAH,LCRYST,AO,KM,DX                            JOB,171
      WRITE (6,9720)                                                    JOB,172
 9720 FORMAT(////,30X,5H  ION,/,30X,40H  ENERGY       N(100)    N(110)
     2 (111) ,//)                                                       JOB,174
      WRITE (6,9730) (EOUT(N),(PEL(N,M),M=1,3),N=1,KEOM)                JOB,175
 9730 FORMAT(26X,F10.0,5X,3F10.5)                                       JOB,176
      WRITE (6,9740) PSE(I),FIT(I)                                      JOB,177
 9740 FORMAT(///30X,20HPSE CONTRIBUTION WAS,F6.3,13H, FIT WAS AT ,F6.3,
     2  14H ELECTRONS/ION  )
 3500 CONTINUE                                                          JOB,180
      GO TO 15                                                          JOB,181
 9999 STOP
      END                                                               JOB,183
      END
//GO.SYSIN DD *
```

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ABSTRACT

This thesis is a computer simulation of secondary electron emission (SEE) from monocrystalline metals and alkali-halides using a modified version of the Harrison, Carlston and Magnuson single collision theory of SEE. Three cases of SEE are investigated: the angular dependence of SEE from Cu bombarded by Ar^{+}, the dependence of SEE as a function of energy for rare gas ions normally incident on the (100), (110) and (111) faces of metal single crystals, and the dependence of SEE as a function of energy for Ar^{+} and Ne^{+} ions normally incident on the (100), (110) and (111) faces of KCl. The theory does not accurately describe the angular dependence of SEE for monocrystalline Cu targets, but does accurately predict the modified sec θ dependence found experimentally in polycrystalline studies. For the metal targets, the difference between the theoretical kinetic secondary emission result and the experimental datum is identified as potential secondary emission. The alkali-halide SEE simulation agrees reasonably well with experiment.

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